## Supplemental Materials and Methods

## Cells, antibodies and reagents

KG-1 cells were cultured in RPMI 1640 supplemented with $10 \%$ fetal calf serum and antibiotics. For SILAC labeling of KG-1 cells ${ }^{13} \mathrm{C}_{6}{ }^{15} \mathrm{~N}_{4}$ L-arginine and ${ }^{13} \mathrm{C}_{6}{ }^{15} \mathrm{~N}_{2}$ L-Lysine (both Cambridge Isotopes, Andover, USA) were used.
Regarding the primary AML cells all patients gave written informed consent. Baseline morphology, cytogenetics and cell surface antigen analysis were performed as part of the routine clinical evaluation. Immunomagnetically enriched CD34 ${ }^{+}$cells were maintained in liquid culture (X-Vivo 10, Lonza, Basel, Switzerland) supplemented with 10\% FBS (HyClone, Perbio, Aalst, Belgium), 1\% L-Glutamin (Gibco, Darmstadt, Germany), interleukin-3, thrombopoietin ( $25 \mathrm{ng} / \mathrm{mL}$ each), stem cell factor and flt-3 ligand ( $50 \mathrm{ng} / \mathrm{mL}$ each, Peprotech, Hamburg, Germany) with medium changes to $2 \times 10^{5}$ cells $/ \mathrm{ml}$ every 7 days.

Antibodies for western-blot analyses recognized (p)Syk(Tyr525/526), SLP65, pTyr(4G10), (p)STAT3(Tyr705), (p)STAT5(Tyr694), Pim1, Socs3 and actin (all from Cell Signaling Technology (Danvers, USA) or Santa Cruz Biotechnology (Santa Cruz, USA)). Antibodies recognizing FcR $\gamma$ were purchased from Millipore (Billerica, USA), the antibodies recognizing CD18 and Mac-1 were purchased from Novus Biologicals (Littleton, USA). For immobilization of antibodies Protein A/G Sepharose was used (Santa Cruz Biotechnology).
The Syk inhibitor Bay 61-3606 (Merck, Darmstadt, Germany) was resuspended in $\mathrm{H}_{2} \mathrm{O}$ and was stored at $-20^{\circ} \mathrm{C}$; it was used in a final concentration of 250 nM . Calf intestinal alkaline phosphatase (CIP (New England Biolabs, Ipswich, USA)) was subjected to cleared cellular lysates for 30 min at $37^{\circ} \mathrm{C}$ for dephosphorylation of proteins in vitro.

## Vectors and cell transduction

Sequences targeted by each Syk shRNA were described previously ${ }^{4}$. shRNAs targeting Syk, FcR $\gamma$-, Mac-1- or CD18 were purchased from Sigma-Aldrich and the shRNA encoding sequences were cloned into pLKO. 1 vectors for lentiviral transduction.
The following shRNA constructs were used: shRNA specific for FcR $\gamma$ : Sigma-TRCN 0000057454. shRNA specific for Mac-1: Sigma-TRCN 0000414619. shRNA specific for CD18: Sigma-TRCN 0000029643. Cloning of the oligonucleotides and cell infections were performed as described previously ${ }^{4}$. The retroviral vectors pMSCV-iGFP, pMSCV-iGFPcaSTAT3 and pMSCV-iGFP-caSTAT5A were kindly provided by C. Wichmann and R. Moriggl. The STAT3 cDNA was manipulated by site-directed mutagenesis in a way that upon expression cysteine residues substituted A661 and N663 of STAT3 ${ }^{22}$. The cDNA encoding for constitutively active STAT5A harbors point mutations resulting in the replacement of S711 by phenylalanine on the protein leve ${ }^{23}$. Retroviral transductions were performed as described previously ${ }^{24}$.

## Mass spectrometric analysis, database search and MaxQuant-based protein quantification

All slices were reduced with 10 mM DTT for 55 min at $56^{\circ} \mathrm{C}$, alkylated with 55 mM IAA for 20 min at $26^{\circ} \mathrm{C}$ and digested with modified trypsin (Promega, Madison, USA) overnight at $37^{\circ} \mathrm{C}$. Tryptic peptides were injected into a $\mathrm{C}_{18}$ precolumn ( $1.5 \mathrm{~cm}, 360 \mu \mathrm{~m}$ o.d., $150 \mu \mathrm{~m}$ i.d., Reprosil-Pur $120 \mathrm{~A}^{\circ}, 3 \mu \mathrm{~m}, \mathrm{C}_{18}-\mathrm{AQ}$, Dr Maisch GmbH ) at a flow rate of $10 \mathrm{ml} / \mathrm{min}$. Bound peptides were eluted and separated on a $\mathrm{C}_{18}$ capillary column ( $15 \mathrm{~cm}, 360 \mu \mathrm{~m}$ o.d., $75 \mu \mathrm{~m}$ i.d., Reprosil-Pur $120 A^{\circ}, 3 \mu \mathrm{~m}, \mathrm{C}_{18}-\mathrm{AQ}$, Dr Maisch GmbH ) at a flow rate of $300 \mathrm{nl} / \mathrm{min}$, with a gradient from 7.5 to $37.5 \%$ ACN in $0.1 \%$ formic acid for 50 min using an Agilent 1100 nanoflow LC system (Agilent Technologies, Böblingen, Germany) coupled to an LTQ-Orbitrap XL hybrid mass spectrometer (Thermo Fisher Scientific, Waltham, USA). MS conditions were as followed: spray voltage, 1.6 kV ; heated capillary temperature, $150^{\circ} \mathrm{C}$; normalized collisioninduced dissociation (CID) collision energy 37.5\% for MS/MS in LTQ. An activation q=0.25 and activation time of 30 ms were used. The mass spectrometer was operated in the datadependent mode to automatically switch between MS and MS/MS acquisition. Survey MS spectra were acquired in the Orbitrap ( $\mathrm{m} / \mathrm{z} 350-1600$ ) with the resolution set to 30000 at $\mathrm{m} / \mathrm{z}$ 400 and automatic gain control target at $5 \times 10^{5}$. The five most intense ions were sequentially isolated for CID MS/MS fragmentation and detection in the linear ion trap. Ions with single and unrecognized charge states were excluded. Raw data were analysed with MaxQuant software (Version 1.0.13.13) in combination with Mascot search engine for peptide and protein identifications (Version 2.2.07, Matrix Science). IPI human database (Version 3.87) was used as human sequence database. MS/MS peak lists were filtered to contain at most six peaks per 100 Da interval and searched against Mascot server. The MS mass tolerance was set to 7 ppm and MS/MS mass tolerance was set to 0.6 Da . Up to three missed cleavages of trypsin were allowed. Oxidized methionine and cysteine carbamido-methylation were searched as variable modifications. The modifications corresponding to arginine and lysine labeled with heavy stable isotopes were handled as fixed modifications in the Mascot search, if applicable, after identification of SILAC pairs by MaxQuant. The false positive rate was set to $1 \%$ at the peptide level, the false discovery rate was set to $1 \%$ at the protein level and the minimum required peptide length was set to six amino acids.

## Mass spectrometric phosphopeptide analysis

The Syk band was excised, reduced, alkylated, in-gel digested with trypsin, and then extracted from the gel, as described above. The tryptic peptides were re-dissolved in $20 \mu \mathrm{l}$

DHB solution (200mg 2,5-dihydroxybenzoic acid (Sigma, USA) in 1 ml of $80 \%$ acetonitrile, $5 \%$ trifluoroacetic acid and loaded onto a $\mathrm{TiO}_{2}$ microcolumn (GL Sciences Inc.), as described ${ }^{19}$. The columns were washed three times with $20 \mu$ I DHB solution and five times with $20 \mu$ l of a solution of $5 \%$ trifluoroacetic acid and $80 \%$ acetonitrile to remove non-specific binding peptides and DHB. The bound peptides were then eluted with $3 \times 20 \mu \mathrm{l}$ of 0.3 N $\mathrm{NH}_{4} \mathrm{OH}(\mathrm{pH}>10.5)$ and evaporated to dryness in a SpeedVac for further MS analysis. The LTQ-Orbitrap Velos hybrid mass spectrometer (Thermo Fisher Scientific, Waltham, USA) was used in place of LTQ-Orbitrap XL hybrid mass spectrometer. The multistage activation of neutral loss of phosphoric acid was used in all CID MS/MS events to improve the fragmentation spectra of the phosphopeptides. All MS/MS spectra were searched using MASCOT v2.2.07 against the IPI human database (Version 3.87) with the following criteria: peptide mass tolerance, 10 ppm ; MS/MS ion mass tolerance, 0.6 Da ; number of missed cleavages allowed, up to three. The variable modifications considered were phosphorylation of serine, threonine and tyrosine, methionine oxidation, and cysteine carboxyamidomethylation. All phosphorylated sites were examined manually by the presence of a mass difference of 69 Da between fragment ions for phosphoserine and a difference of 83 Da for phosphothreonine (supplementary table 1, supplementary figure 1).

## Cell proliferation assay

$5 \cdot 10^{3}$ FFM 05 or FFM12, or $10^{3} \mathrm{KG}-1$ cells were seeded into the wells of a 96 -well plate on day zero. The cells were cultured in the respective growth media outlined above. At given time points the cells were treated using a mixture consisting of the XTT-labeling reagent and the electron coupling reagent according to the protocol of the cell proliferation kit II (Roche). Four hours later the XTT-derived signals that are proportional to the cell numbers were monitored by an Elisa-Reader (Spectra Fluor Plus, specific absorbance filter: 475nm, nonspecific absorbance filter: 660nm) (Tecan). Wells containing groth media served as background controls in all experiments. In case of AML cell/stroma co-culture experiments, wells containing stroma cells and growth media were used as background controls.

## In vitro kinase assays

For phosphorylation the recombinant catalytic domain of Syk (Biomol, Germany) was used or Syk was purified by immunopurification as described above and resuspended in kinase buffer containing 60 mM HEPES $\mathrm{pH} 7.5 ; 5 \mathrm{mM} \mathrm{MgCL} 2 ; 5 \mathrm{mM} \mathrm{MnCL} ; 2 \mu \mathrm{M} \mathrm{Na} 3{ }_{2} \mathrm{VO}_{4} ; 1.25 \mathrm{mM}$ DTT. Protein A/G beads only served as negative control for the immunopurification. $1.5 \mu \mathrm{M}$ biotinylated substrate peptide and $20 \mu \mathrm{M}$ ATP were added, incubated for 15 min at $37^{\circ} \mathrm{C}$, and the reaction was stopped by adding EDTA to a final concentration of 25 mM . Peptides were immobilized on streptavidine-coated 96well plates (Millipore, Billerica, USA) and
phosphorylation efficiency was determined by ELISA using $1 \mu \mathrm{~g} / \mathrm{ml}$ anti-pTyr (Millipore, Billerica, USA) and 1:1000 HRPO-conjugated anti-mouse IgG antibodies (Pierce, Rockford, USA). The mean value and standard deviation (SD) of quadruplicates was determined by calculating the difference of absorption at 405 nm and background absorption at 490 nm .

| Sequence | Modification | Exp. m/z | Exp <br> M.W. | Charge | Delta | Mascot lon score |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| (R)ADENYyK(A) | pY | 491.6796 | 981.345 | 2 | -0.003 | 27.0 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | $\mathrm{B}-\mathrm{NH} 3$ | $\mathrm{~B}-\mathrm{H} 2 \mathrm{O}$ | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y -NH3 | $\mathrm{Y}+\mathrm{H} 2 \mathrm{O}$ | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 72.0 |  |  |  | A | 982.4 | 491.7 | 965.3 | 964.3 | 7 |
| 2 | 187.1 |  |  | 169.1 | D | 911.3 | 456.2 | 894.3 | 893.3 | 6 |
| 3 | 316.1 |  |  | 298.1 | E | 796.3 |  | 779.3 | 778.3 | 5 |
| 4 | 430.2 |  | 413.1 | 412.1 | N | 667.2 |  | 650.2 |  | 4 |
| 5 | 593.2 |  | 576.2 | 575.2 | Y | 553.2 |  | 536.2 |  | 3 |
| 6 | 836.2 | 418.6 | 819.2 | 818.2 | Y+80 | 390.1 |  | 373.1 |  | 2 |
| 7 | 982.4 | 491.7 | 965.3 | 964.3 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp <br> M.W. | Charge | Delta | Mascot lon score |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| (R)ADENyYK(A) | pY | 491.6810 | 981.347 | 2 | -0.001 | 33.0 |



| B | B Ions | B+2H | B-NH3 | B-H2O | AA | Y Ions | $Y+2 H$ | $Y-N H 3$ | $Y-H 2 O$ | $Y$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 72.0 |  |  |  | A | 982.4 | 491.7 | 965.3 | 964.3 | 7 |
| 2 | 187.1 |  |  | 169.1 | D | 911.3 | 456.2 | 894.3 | 893.3 | 6 |
| 3 | 316.1 |  |  | 298.1 | E | 796.3 |  | 779.3 | 778.3 | 5 |
| 4 | 430.2 |  | 413.1 | 412.1 | N | 667.2 |  | 650.2 |  | 4 |
| 5 | 673.2 |  | 656.2 | 655.2 | Y+80 | 553.2 |  | 536.2 |  | 3 |
| 6 | 836.2 | 418.6 | 819.2 | 818.2 | Y | 310.2 |  | 293.1 |  | 2 |
| 7 | 982.4 | 491.7 | 965.3 | 964.3 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp <br> M.W. | Charge | Delta | Mascot lon score |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| (K)ALRADENyyK(A) | pY, pY | 701.7742 | 1401.534 | 2 | -0.003 | 28.2 |



| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | $Y$ Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 72.0 |  |  |  | A | 1,402.5 | 701.8 | 1,385.5 | 1,384.5 | 10 |
| 2 | 185.1 |  |  |  | L | 1,331.5 | 666.3 | 1,314.5 | 1.313.5 | 9 |
| 3 | 341.2 | 171.1 | 324.2 |  | R | 1.218.4 | 609.7 | 1,201.4 | 1,200.4 | 8 |
| 4 | 412.3 | 206.6 | 395.2 |  | A | 1.062.3 | 531.7 | 1,045.3 | 1.044.3 | 7 |
| 5 | 527.3 | 264.2 | 510.3 | 509.3 | D | 991.3 | 496.1 | 974.3 | 973.3 | 6 |
| 6 | 656.3 | 328.7 | 639.3 | 638.3 | E | 876.3 |  | 859.2 | 858.2 | 5 |
| 7 | 770.4 | 385.7 | 753.4 | 752.4 | N | 747.2 |  | 730.2 |  | 4 |
| 8 | 1.013.4 | 507.2 | 996.4 | 995.4 | $\mathbf{Y + 8 0}$ | 633.2 |  | 616.1 |  | 3 |
| 9 | 1.256.4 | 628.7 | 1,239.4 | 1.238.4 | Y+80 | 390.1 |  | 373.1 |  | 2 |
| 10 | 1,402.5 | 701.8 | 1,385.5 | 1,384.5 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp <br> M.W. | Charge | Delta | Mascot lon score |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| (K)ALRADENyYK(A) | pY | 441.5302 | 1321.569 | 3 | -0.002 | 25.7 |



| B | B Ions | B $+2 H$ | B-NH3 | B-H2O | AA | Y Ions | $Y+2 H$ | $Y-N H 3$ | $Y-H 2 O$ | $Y$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 72.0 |  |  |  | A | $\mathbf{1 , 3 2 2 . 6}$ | 661.8 | $\mathbf{1 . 3 0 5 . 6}$ | $\mathbf{1 . 3 0 4 . 6}$ | 10 |
| 2 | 185.1 |  |  |  | L | $\mathbf{1 . 2 5 1 . 5}$ | 626.3 | $\mathbf{1 . 2 3 4 . 5}$ | $\mathbf{1 . 2 3 3 . 5}$ | 9 |
| 3 | 341.2 | $\mathbf{1 7 1 . 1}$ | 324.2 |  | R | $\mathbf{1 . 1 3 8 . 5}$ | 569.7 | $\mathbf{1 . 1 2 1 . 4}$ | $\mathbf{1 . 1 2 0 . 4}$ | 8 |
| 4 | 412.3 | 206.6 | 395.2 |  | A | 982.4 | 491.7 | 965.3 | 964.3 | 7 |
| 5 | 527.3 | 264.2 | 510.3 | 509.3 | D | 911.3 | 456.2 | 894.3 | 893.3 | 6 |
| 6 | 656.3 | 328.7 | 639.3 | 638.3 | E | 796.3 |  | 779.3 | 778.3 | 5 |
| 7 | 770.4 | 385.7 | 753.4 | 752.4 | N | 667.2 |  | 650.2 |  | 4 |
| 8 | 1.013 .4 | 507.2 | 996.4 | 995.4 | Y+80 | 553.2 |  | 536.2 |  | 3 |
| 9 | $\mathbf{1 . 1 7 6 . 5}$ | 588.7 | $\mathbf{1 . 1 5 9 . 4}$ | $\mathbf{1 . 1 5 8 . 5}$ | Y | 310.2 |  | 293.1 |  | 2 |
| 10 | $\mathbf{1 . 3 2 2 . 6}$ | 661.8 | $\mathbf{1 . 3 0 5 . 6}$ | $\mathbf{1 . 3 0 4 . 6}$ | K | $\mathbf{1 4 7 . 1}$ |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp <br> M.W. | Charge | Delta | Mascot lon score |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| (R)DNNGsYALCLLHEGK(V) | pS | 857.3626 | 1712.711 | 2 | -0.012 | 43.2 |



| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | $Y$ Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 116.0 |  |  | 98.0 | D | 1,713.7 | 857.4 | 1,696.7 | 1.695 .7 | 15 |
| 2 | 230.1 |  | 213.1 | 212.1 | N | 1,598.7 | 799.9 | 1,581.7 | 1,580.7 | 14 |
| 3 | 344.1 |  | 327.1 | 326.1 | N | 1,484.7 | 742.8 | 1,467.6 | 1,466.6 | 13 |
| 4 | 401.1 |  | 384.1 | 383.1 | G | 1,370.6 | 685.8 | 1,353.6 | 1,352.6 | 12 |
| 5 | 568.1 |  | 551.1 | 550.1 | S+80 | 1,313.6 | 657.3 | 1.296 .6 | 1.295.6 | 11 |
| 6 | 731.2 | 366.1 | 714.2 | 713.2 | Y | 1.146.6 | 573.8 | 1.129.6 | 1.128.6 | 10 |
| 7 | 802.2 | 401.6 | 785.2 | 784.2 | A | 983.5 | 492.3 | 966.5 | 965.5 | 9 |
| 8 | 915.3 | 458.2 | 898.3 | 897.3 | L | 912.5 | 456.8 | 895.5 | 894.5 | 8 |
| 9 | 1.018.3 | 509.7 | 1,001.3 | 1,000.3 | C | 799.4 | 400.2 | 782.4 | 781.4 | 7 |
| 10 | 1,131.4 | 566.2 | 1.114.4 | 1,113.4 | L | 696.4 | 348.7 | 679.4 | 678.4 | 6 |
| 11 | 1,244.5 | 622.8 | 1,227.5 | 1,226.5 | L | 583.3 | 292.2 | 566.3 | 565.3 | 5 |
| 12 | 1,381.6 | 691.3 | 1,364.5 | 1,363.6 | H | 470.2 | 235.6 | 453.2 | 452.2 | 4 |
| 13 | 1,510.6 | 755.8 | 1,493.6 | 1.492 .6 | E | 333.2 |  | 316.2 | 315.2 | 3 |
| 14 | 1,567.6 | 784.3 | 1,550.6 | 1,549.6 | G | 204.1 |  | 187.1 |  | 2 |
| 15 | 1,713.7 | 857.4 | 1,696.7 | 1,695.7 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. $\mathrm{m} / \mathrm{z}$ | Exp <br> M.W. | Charge | Delta | Mascot lon score |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $(\mathrm{R})$ EALPmDTEVYEsPyADPEEIRPK(E) | Mox, pS, pY | 952.3954 | 2854.164 | 3 | -0.006 | 34.0 |



| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | $Y$ Ions | $Y+2 \mathrm{H}$ | Y -NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 130.0 |  |  | 112.0 | E | 2.855 .2 | 1,428.1 | 2,838.2 | 2,837.2 | 23 |
| 2 | 201.1 |  |  | 183.1 | A | 2.726 .1 | 1,363.6 | 2,709.1 | 2,708.1 | 22 |
| 3 | 314.2 |  |  | 296.2 | L | 2.655 .1 | 1.328.1 | 2,638.1 | $2,637.1$ | 21 |
| 4 | 411.2 |  |  | 393.2 | P | 2,542.0 | 1.271.5 | 2,525.0 | 2,524.0 | 20 |
| 5 | 558.3 |  |  | 540.2 | M+16 | 2,445.0 | 1.223 .0 | 2,427.9 | 2,427.0 | 19 |
| 6 | 673.3 | 337.1 |  | 655.3 | D | 2,297.9 | 1.149.5 | 2,280.9 | 2,279.9 | 18 |
| 7 | 774.3 | 387.7 |  | 756.3 | T | 2,182.9 | 1.092 .0 | 2,165.9 | 2,164.9 | 17 |
| 8 | 903.4 | 452.2 |  | 885.4 | E | 2,081.9 | 1.041.4 | 2,064.8 | 2,063.8 | 16 |
| 9 | 1,002.4 | 501.7 |  | 984.4 | V | 1.952 .8 | 976.9 | 1,935.8 | 1.934 .8 | 15 |
| 10 | 1,165.5 | 583.3 |  | 1.147.5 | Y | 1,853.7 | 927.4 | 1,836.7 | 1,835.7 | 14 |
| 11 | 1,294.6 | 647.8 |  | 1,276.5 | E | 1,690.7 | 845.8 | 1.673 .6 | 1,672.7 | 13 |
| 12 | 1.461.5 | 731.3 |  | 1,443.5 | S+80 | 1,561.6 | 781.3 | 1,544.6 | 1,543.6 | 12 |
| 13 | 1,558.6 | 779.8 |  | 1.540 .6 | P | 1.394 .6 | 697.8 | 1,377.6 | 1,376.6 | 11 |
| 14 | 1.801.6 | 901.3 |  | 1.783 .6 | Y+80 | 1,297.6 | 649.3 | 1,280.6 | 1,279.6 | 10 |
| 15 | 1.872.7 | 936.8 |  | 1,854.7 | A | 1,054.6 | 527.8 | 1,037.5 | 1,036.5 | 9 |
| 16 | 1,987.7 | 994.4 |  | 1.969.7 | D | 983.5 | 492.3 | 966.5 | 965.5 | 8 |
| 17 | 2,084.7 | 1,042.9 |  | 2,066.7 | P | 868.5 | 434.7 | 851.5 | 850.5 | 7 |
| 18 | 2,213.8 | 1,107.4 |  | 2,195.8 | E | 771.4 | 386.2 | 754.4 | 753.4 | 6 |
| 19 | 2,342.8 | 1,171.9 |  | 2,324.8 | E | 642.4 | 321.7 | 625.4 | 624.4 | 5 |
| 20 | 2,455.9 | 1.228.5 |  | 2,437.9 | I | 513.4 | 257.2 | 496.3 |  | 4 |
| 21 | 2,612.0 | 1.306.5 | 2,595.0 | 2,594.0 | R | 400.3 | 200.6 | 383.2 |  | 3 |
| 22 | 2,709.1 | 1,355.0 | 2,692.0 | 2,691.1 | P | 244.2 |  | 227.1 |  | 2 |
| 23 | 2,855.2 | 1,428.1 | 2,838.2 | 2,837.2 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. $\mathrm{m} / \mathrm{z}$ | Exp <br> M.W. | Charge | Delta | Mascot lon score |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $(\mathrm{R})$ EALPmDTEVyESPyADPEEIRPK(E) | Mox, pY, pY | 952.3952 | 2854.164 | 3 | -0.006 | 53.5 |



| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | $Y$ Ions | $Y+2 \mathrm{H}$ | Y-NH3 | Y- H 2 O | $Y$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 130.0 |  |  | 112.0 | E | 2.855 .2 | 1,428.1 | 2,838.2 | 2,837.2 | 23 |
| 2 | 201.1 |  |  | 183.1 | A | 2,726.1 | 1,363.6 | 2,709.1 | 2,708.1 | 22 |
| 3 | 314.2 |  |  | 296.2 | L | 2,655.1 | 1.328.1 | 2,638.1 | 2,637.1 | 21 |
| 4 | 411.2 |  |  | 393.2 | P | 2,542.0 | 1.271 .5 | 2,525.0 | 2,524.0 | 20 |
| 5 | 558.3 |  |  | 540.2 | M+16 | 2,445.0 | 1.223.0 | 2,427.9 | 2.427 .0 | 19 |
| 6 | 673.3 | 337.1 |  | 655.3 | D | 2,297.9 | 1.149.5 | 2,280.9 | 2,279.9 | 18 |
| 7 | 774.3 | 387.7 |  | 756.3 | T | 2,182.9 | 1.092 .0 | 2,165.9 | 2,164.9 | 17 |
| 8 | 903.4 | 452.2 |  | 885.4 | E | 2,081.9 | 1.041.4 | 2,064.8 | 2,063.8 | 16 |
| 9 | 1.002.4 | 501.7 |  | 984.4 | V | 1.952 .8 | 976.9 | 1.935 .8 | 1,934.8 | 15 |
| 10 | 1.245 .5 | 623.2 |  | 1.227.5 | $\mathbf{Y}+80$ | 1,853.7 | 927.4 | 1,836.7 | 1,835.7 | 14 |
| 11 | 1.374.5 | 687.8 |  | 1,356.5 | E | 1.610.7 | 805.9 | 1.593.7 | 1,592.7 | 13 |
| 12 | 1.461.5 | 731.3 |  | 1,443.5 | 5 | 1.481 .7 | 741.3 | 1,464.6 | 1,463.7 | 12 |
| 13 | 1.558.6 | 779.8 |  | 1.540 .6 | P | 1.394 .6 | 697.8 | 1,377.6 | 1,376.6 | 11 |
| 14 | 1.801.6 | 901.3 |  | 1.783 .6 | $\mathbf{Y}+80$ | 1.297 .6 | 649.3 | 1,280.6 | 1,279.6 | 10 |
| 15 | 1.872.7 | 936.8 |  | 1,854.7 | A | 1.054.6 | 527.8 | 1,037.5 | 1,036.5 | 9 |
| 16 | 1.987 .7 | 994.4 |  | 1.969.7 | D | 983.5 | 492.3 | 966.5 | 965.5 | 8 |
| 17 | 2,084.7 | 1.042.9 |  | 2,066.7 | P | 868.5 | 434.7 | 851.5 | 850.5 | 7 |
| 18 | 2,213.8 | 1.107.4 |  | 2,195.8 | E | 771.4 | 386.2 | 754.4 | 753.4 | 6 |
| 19 | 2,342.8 | 1.171.9 |  | 2,324.8 | E | 642.4 | 321.7 | 625.4 | 624.4 | 5 |
| 20 | 2,455.9 | 1.228.5 |  | 2.437 .9 | I | 513.4 | 257.2 | 496.3 |  | 4 |
| 21 | 2,612.0 | 1.306.5 | 2,595.0 | 2,594.0 | R | 400.3 | 200.6 | 383.2 |  | 3 |
| 22 | 2,709.1 | 1,355.0 | 2,692.0 | 2,691.1 | P | 244.2 |  | 227.1 |  | 2 |
| 23 | 2,855.2 | 1,428.1 | 2,838.2 | 2,837.2 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp <br> M.W. | Charge | Delta | Mascot lon score |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $(R)$ EALPmDTEVyESPYADPEEIRPK(E) | Mox, pY | 925.7402 | 2774.199 | 3 | -0.005 | 58.6 |



| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | $Y$ Ions | $Y+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 130.0 |  |  | 112.0 | E | $2,775.2$ | 1,388.1 | 2,758.2 | 2,757.2 | 23 |
| 2 | 201.1 |  |  | 183.1 | A | 2,646.2 | 1,323.6 | 2,629.1 | 2,628.2 | 22 |
| 3 | 314.2 |  |  | 296.2 | L | 2,575.1 | 1.288.1 | 2,558.1 | 2,557.1 | 21 |
| 4 | 411.2 |  |  | 393.2 | P | 2,462.0 | 1.231.5 | 2,445.0 | 2,444.0 | 20 |
| 5 | 558.3 |  |  | 540.2 | M+16 | 2,365.0 | 1.183.0 | 2,348.0 | 2,347.0 | 19 |
| 6 | 673.3 | 337.1 |  | 655.3 | D | 2.218 .0 | 1.109.5 | 2,200.9 | 2,199.9 | 18 |
| 7 | 774.3 | 387.7 |  | 756.3 | T | 2,102.9 | 1.052 .0 | 2,085.9 | 2,084.9 | 17 |
| 8 | 903.4 | 452.2 |  | 885.4 | E | 2,001.9 | 1.001.4 | 1,984.9 | 1,983.9 | 16 |
| 9 | 1.002.4 | 501.7 |  | 984.4 | V | 1,872.8 | 936.9 | 1,855.8 | 1.854 .8 | 15 |
| 10 | 1.245 .5 | 623.2 |  | 1,227.5 | $\mathbf{Y}+80$ | 1,773.8 | 887.4 | 1,756.7 | 1.755 .8 | 14 |
| 11 | 1,374.5 | 687.8 |  | 1,356.5 | E | 1,530.7 | 765.9 | 1,513.7 | 1,512.7 | 13 |
| 12 | 1.461.5 | 731.3 |  | 1,443.5 | 5 | 1,401.7 | 701.4 | 1,384.7 | 1,383.7 | 12 |
| 13 | 1.558.6 | 779.8 |  | 1.540 .6 | P | 1.314.7 | 657.8 | 1.297 .6 | 1.296 .7 | 11 |
| 14 | 1,721.7 | 861.3 |  | 1,703.7 | Y | 1.217 .6 | 609.3 | 1,200.6 | 1.199.6 | 10 |
| 15 | 1,792.7 | 896.9 |  | 1.774 .7 | A | 1,054.6 | 527.8 | 1,037.5 | 1,036.5 | 9 |
| 16 | 1.907 .7 | 954.4 |  | 1.889 .7 | D | 983.5 | 492.3 | 966.5 | 965.5 | 8 |
| 17 | 2,004.8 | 1.002 .9 |  | $1,986.8$ | P | 868.5 | 434.7 | 851.5 | 850.5 | 7 |
| 18 | 2,133.8 | 1.067.4 |  | 2,115.8 | E | 771.4 | 386.2 | 754.4 | 753.4 | 6 |
| 19 | 2,262.9 | 1.131.9 |  | 2,244.9 | E | 642.4 | 321.7 | 625.4 | 624.4 | 5 |
| 20 | 2,376.0 | 1,188.5 |  | 2,357.9 | I | 513.4 | 257.2 | 496.3 |  | 4 |
| 21 | 2,532.1 | 1.266.5 | 2.515 .0 | 2,514.0 | R | 400.3 | 200.6 | 383.2 |  | 3 |
| 22 | 2,629.1 | 1,315.1 | 2,612.1 | 2,611.1 | P | 244.2 |  | 227.1 |  | 2 |
| 23 | 2,775.2 | 1,388.1 | 2,758.2 | 2,757.2 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp <br> M.W. | Charge | Delta | Mascot lon score |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| (R)EALPmDTEVYEsPYADPEEIRPK(E) | Mox, pS | 925.7404 | 2774.199 | 3 | -0.004 | 61.4 |



| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | $\mathrm{B}-\mathrm{NH} 3$ | B- $\mathrm{H}_{2} \mathrm{O}$ | AA | $Y$ Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y H 2 O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 130.0 |  |  | 112.0 | E | 2.775 .2 | 1,388.1 | 2.758 .2 | 2.757 .2 | 23 |
| 2 | 201.1 |  |  | 183.1 | A | 2,646.2 | 1,323.6 | 2.629 .1 | 2.628 .2 | 22 |
| 3 | 314.2 |  |  | 296.2 | L | 2,575.1 | 1.288.1 | 2,558.1 | 2,557.1 | 21 |
| 4 | 411.2 |  |  | 393.2 | P | 2,462.0 | 1.231 .5 | 2,445.0 | 2,444.0 | 20 |
| 5 | 558.3 |  |  | 540.2 | M+16 | 2,365.0 | 1.183.0 | 2,348.0 | 2,347.0 | 19 |
| 6 | 673.3 | 337.1 |  | 655.3 | D | 2.218 .0 | 1.109 .5 | 2,200.9 | 2,199.9 | 18 |
| 7 | 774.3 | 387.7 |  | 756.3 | T | 2,102.9 | 1.052 .0 | 2,085.9 | 2,084.9 | 17 |
| 8 | 903.4 | 452.2 |  | 885.4 | E | 2,001.9 | 1.001.4 | 1,984.9 | 1,983.9 | 16 |
| 9 | 1.002.4 | 501.7 |  | 984.4 | V | 1.872 .8 | 936.9 | 1.855 .8 | 1.854 .8 | 15 |
| 10 | 1,165.5 | 583.3 |  | 1.147.5 | Y | 1.773.8 | 887.4 | 1,756.7 | 1.755.8 | 14 |
| 11 | 1,294.6 | 647.8 |  | 1.276.5 | E | 1.610 .7 | 805.9 | 1.593.7 | 1.592 .7 | 13 |
| 12 | 1.461.5 | 731.3 |  | 1,443.5 | $5+80$ | 1.481 .7 | 741.3 | 1,464.6 | 1,463.7 | 12 |
| 13 | 1,558.6 | 779.8 |  | 1.540 .6 | P | 1.314 .7 | 657.8 | 1,297.6 | 1.296 .7 | 11 |
| 14 | 1.721 .7 | 861.3 |  | 1,703.7 | Y | 1.217 .6 | 609.3 | 1,200.6 | 1.199.6 | 10 |
| 15 | 1.792 .7 | 896.9 |  | 1,774.7 | A | 1.054.6 | 527.8 | 1,037.5 | 1.036.5 | 9 |
| 16 | 1.907 .7 | 954.4 |  | 1.889.7 | D | 983.5 | 492.3 | 966.5 | 965.5 | 8 |
| 17 | 2,004.8 | 1,002.9 |  | 1.986 .8 | P | 868.5 | 434.7 | 851.5 | 850.5 | 7 |
| 18 | 2,133.8 | 1.067.4 |  | 2,115.8 | E | 771.4 | 386.2 | 754.4 | 753.4 | 6 |
| 19 | 2,262.9 | 1.131.9 |  | 2,244.9 | E | 642.4 | 321.7 | 625.4 | 624.4 | 5 |
| 20 | 2,376.0 | 1.188 .5 |  | 2,357.9 | I | 513.4 | 257.2 | 496.3 |  | 4 |
| 21 | 2.532 .1 | 1.266 .5 | 2.515 .0 | 2,514.0 | R | 400.3 | 200.6 | 383.2 |  | 3 |
| 22 | 2.629 .1 | 1,315.1 | 2.612 .1 | 2.611 .1 | P | 244.2 |  | 227.1 |  | 2 |
| 23 | 2,775.2 | 1,388.1 | 2,758.2 | 2.757 .2 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp <br> M.W. | Charge | Delta | Mascot lon score |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| (R)EALPMDTEVYESPYADPEEIRPK(E) | pY | 920.4084 | 2758.203 | 3 | -0.005 | 72.4 |



| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B H 2 O | AA | $Y$ Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 130.0 |  |  | 112.0 | E | 2,759.2 | 1.380 .1 | 2,742.2 | 2,741.2 | 23 |
| 2 | 201.1 |  |  | 183.1 | A | $2,630.2$ | 1,315.6 | 2,613.1 | 2,612.2 | 22 |
| 3 | 314.2 |  |  | 296.2 | L | 2,559.1 | 1.280.1 | 2,542.1 | 2,541.1 | 21 |
| 4 | 411.2 |  |  | 393.2 | P | 2,446.1 | 1.223 .5 | 2,429.0 | 2,428.0 | 20 |
| 5 | 542.3 |  |  | 524.3 | M | 2,349.0 | 1.175.0 | 2,332.0 | 2,331.0 | 19 |
| 6 | 657.3 | 329.1 |  | 639.3 | D | 2,218.0 | 1.109.5 | 2,200.9 | 2,199.9 | 18 |
| 7 | 758.3 | 379.7 |  | 740.3 | T | 2,102.9 | 1.052 .0 | 2,085.9 | 2.084 .9 | 17 |
| 8 | 887.4 | 444.2 |  | 869.4 | E | 2,001.9 | 1.001.4 | 1,984.9 | 1,983.9 | 16 |
| 9 | 986.5 | 493.7 |  | 968.4 | V | 1.872 .8 | 936.9 | 1.855 .8 | 1.854 .8 | 15 |
| 10 | 1.149.5 | 575.3 |  | 1.131.5 | Y | 1.773 .8 | 887.4 | 1,756.7 | 1.755 .8 | 14 |
| 11 | 1.278 .6 | 639.8 |  | 1.260.5 | E | 1.610 .7 | 805.9 | 1,593.7 | 1,592.7 | 13 |
| 12 | 1,365.6 | 683.3 |  | 1.347 .6 | 5 | 1.481 .7 | 741.3 | 1.464 .6 | 1,463.7 | 12 |
| 13 | 1,462.6 | 731.8 |  | 1,444.6 | P | 1.394 .6 | 697.8 | 1,377.6 | 1,376.6 | 11 |
| 14 | 1,705.7 | 853.3 |  | 1.687 .7 | Y+80 | 1.297 .6 | 649.3 | 1.280 .6 | 1,279.6 | 10 |
| 15 | 1.776.7 | 888.9 |  | 1,758.7 | A | 1,054.6 | 527.8 | 1,037.5 | 1.036.5 | 9 |
| 16 | 1.891 .7 | 946.4 |  | 1.873 .7 | D | 983.5 | 492.3 | 966.5 | 965.5 | 8 |
| 17 | 1.988.8 | 994.9 |  | 1.970 .8 | P | 868.5 | 434.7 | 851.5 | 850.5 | 7 |
| 18 | 2,117.8 | 1.059.4 |  | 2,099.8 | E | 771.4 | 386.2 | 754.4 | 753.4 | 6 |
| 19 | 2,246.9 | 1,123.9 |  | 2.228 .9 | E | 642.4 | 321.7 | 625.4 | 624.4 | 5 |
| 20 | 2,360.0 | 1.180.5 |  | 2,341.9 | I | 513.4 | 257.2 | 496.3 |  | 4 |
| 21 | 2,516.1 | 1.258.5 | 2,499.0 | 2,498.0 | R | 400.3 | 200.6 | 383.2 |  | 3 |
| 22 | 2,613.1 | 1,307.1 | 2,596.1 | 2,595.1 | P | 244.2 |  | 227.1 |  | 2 |
| 23 | 2,759.2 | 1,380.1 | 2,742.2 | 2,741.2 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp <br> M.W. | Charge | Delta | Mascot lon score |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $(R)$ EESEQIVLIGsK(T) | pS | 706.3378 | 1410.661 | 2 | -0.003 | 30.3 |



| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B H 2 O | AA | $Y$ Ions | Y +2 H | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 130.0 |  |  | 112.0 | E | 1,411.7 | 706.3 | 1,394.6 | 1,393.7 | 12 |
| 2 | 259.1 |  |  | 241.1 | E | 1,282.6 | 641.8 | 1,265.6 | 1,264.6 | 11 |
| 3 | 346.1 |  |  | 328.1 | 5 | 1.153.6 | 577.3 | 1.136 .6 | 1.135 .6 | 10 |
| 4 | 475.2 |  |  | 457.2 | E | 1.066.6 | 533.8 | 1,049.5 | 1,048.5 | 9 |
| 5 | 603.2 |  | 586.2 | 585.2 | Q | 937.5 | 469.3 | 920.5 | 919.5 | 8 |
| 6 | 716.3 | 358.7 | 699.3 | 698.3 | I | 809.5 | 405.2 | 792.4 | 791.4 | 7 |
| 7 | 815.4 | 408.2 | 798.4 | 797.4 | V | 696.4 | 348.7 | 679.3 | 678.4 | 6 |
| 8 | 928.5 | 464.7 | 911.4 | 910.5 | L | 597.3 |  | 580.3 | 579.3 | 5 |
| 9 | 1.041.5 | 521.3 | 1,024.5 | 1.023.5 | I | 484.2 |  | 467.2 | 466.2 | 4 |
| 10 | 1.098.6 | 549.8 | 1,081.5 | 1.080 .6 | G | 371.1 |  | 354.1 | 353.1 | 3 |
| 11 | 1,265.6 | 633.3 | 1.248.5 | 1,247.6 | S+80 | 314.1 |  | 297.1 | 296.1 | 2 |
| 12 | 1,411.7 | 706.3 | 1,394.6 | 1,393.7 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp <br> M.W. | Charge | Delta | Mascot lon score |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $($ K)ELGSGNFGtVK(K) | pT | 594.7671 | 1187.520 | 2 | -0.003 | 35.4 |



| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | $Y$ Ions | Y +2 H | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 130.0 |  |  | 112.0 | E | 1,188.5 | 594.8 | 1,171.5 | 1.170 .5 | 11 |
| 2 | 243.1 |  |  | 225.1 | L | 1,059.5 | 530.2 | 1,042.5 | 1,041.5 | 10 |
| 3 | 300.2 |  |  | 282.1 | G | 946.4 | 473.7 | 929.4 | 928.4 | 9 |
| 4 | 387.2 |  |  | 369.2 | 5 | 889.4 | 445.2 | 872.4 | 871.4 | 8 |
| 5 | 444.2 |  |  | 426.2 | G | 802.3 | 401.7 | 785.3 | 784.3 | 7 |
| 6 | 558.3 | 279.6 | 541.2 | 540.2 | N | 745.3 | 373.2 | 728.3 | 727.3 | 6 |
| 7 | 705.3 | 353.2 | 688.3 | 687.3 | F | 631.3 |  | 614.3 | 613.3 | 5 |
| 8 | 762.3 | 381.7 | 745.3 | 744.3 | G | 484.2 |  | 467.2 | 466.2 | 4 |
| 9 | 943.4 | 472.2 | 926.3 | 925.3 | T+80 | 427.2 |  | 410.2 | 409.2 | 3 |
| 10 | 1.042.4 | 521.7 | 1,025.4 | 1,024.4 | v | 246.2 |  | 229.2 |  | 2 |
| 11 | 1,188.5 | 594.8 | 1.171.5 | 1,170.5 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp <br> M.W. | Charge | Delta | Mascot lon score |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $(R)$ ELNGTyAIAGGR(T) | pY | 651.2977 | 1300.581 | 2 | -0.001 | 53.7 |



| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | $\mathrm{B}-\mathrm{NH} 3$ | B $\mathrm{H}_{2} \mathrm{O}$ | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y H 2 O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 130.0 |  |  | 112.0 | E | 1,301.6 | 651.3 | 1,284.6 | 1,283.6 | 12 |
| 2 | 243.1 |  |  | 225.1 | L | 1,172.5 | 586.8 | 1.155 .5 | 1,154.5 | 11 |
| 3 | 357.2 |  | 340.2 | 339.2 | N | 1.059.5 | 530.2 | 1,042.4 | 1,041.5 | 10 |
| 4 | 414.2 |  | 397.2 | 396.2 | G | 945.4 | 473.2 | 928.4 | 927.4 | 9 |
| 5 | 515.2 |  | 498.2 | 497.2 | T | 888.4 | 444.7 | 871.4 | 870.4 | 8 |
| 6 | 758.3 | 379.6 | 741.2 | 740.3 | $\mathrm{Y}+80$ | 787.3 | 394.2 | 770.3 |  | 7 |
| 7 | 829.3 | 415.2 | 812.3 | 811.3 | A | 544.3 | 272.7 | 527.3 |  | 6 |
| 8 | 942.4 | 471.7 | 925.4 | 924.4 | I | 473.3 |  | 456.3 |  | 5 |
| 9 | 1.013.4 | 507.2 | 996.4 | 995.4 | A | 360.2 |  | 343.2 |  | 4 |
| 10 | 1,070.5 | 535.7 | 1,053.4 | 1.052.4 | G | 289.2 |  | 272.1 |  | 3 |
| 11 | 1.127 .5 | 564.2 | 1,110.5 | 1.109 .5 | G | 232.1 |  | 215.1 |  | 2 |
| 12 | 1,301.6 | 651.3 | 1,284.6 | 1,283.6 | R | 175.1 |  | 158.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp <br> M.W. | Charge | Delta | Mascot lon score |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $(R)$ EMyDLMNLCWTYDVENRPGFAAVELR(L) | pY | 1072.4700 | 3214.388 | 3 | -0.008 | 29.3 |



| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | $Y$ Ions | $Y+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 130.0 |  |  | 112.0 | E | 3,215.4 | 1,608.2 | 3,198.4 | 3,197.4 | 26 |
| 2 | 261.1 |  |  | 243.1 | M | 3,086.4 | 1,543.7 | 3,069.3 | 3,068.4 | 25 |
| 3 | 504.1 |  |  | 486.1 | Y+80 | 2,955.3 | 1.478 .2 | 2,938.3 | 2,937.3 | 24 |
| 4 | 619.1 |  |  | 601.1 | D | 2.712 .3 | 1,356.6 | 2.695 .3 | 2.694 .3 | 23 |
| 5 | 732.2 |  |  | 714.2 | L | 2,597.3 | 1.299.1 | 2,580.2 | 2,579.3 | 22 |
| 6 | 863.3 | 432.1 |  | 845.3 | M | 2,484.2 | 1,242.6 | 2,467.2 | 2,466.2 | 21 |
| 7 | 977.3 | 489.2 | 960.3 | 959.3 | N | 2,353.1 | 1,177.1 | 2,336.1 | 2,335.1 | 20 |
| 8 | 1,090.4 | 545.7 | 1,073.4 | 1,072.4 | L | 2,239.1 | 1,120.1 | 2,222.1 | 2,221.1 | 19 |
| 9 | 1.193.4 | 597.2 | 1,176.4 | 1.175.4 | C | 2,126.0 | 1,063.5 | 2,109.0 | 2,108.0 | 18 |
| 10 | 1.379.5 | 690.2 | 1,362.5 | 1,361.5 | W | 2,023.0 | 1.012.0 | 2,006.0 | 2,005.0 | 17 |
| 11 | 1.480.5 | 740.8 | 1,463.5 | 1,462.5 | T | 1,836.9 | 919.0 | 1,819.9 | 1,818.9 | 16 |
| 12 | 1.643.6 | 822.3 | 1,626.6 | 1.625 .6 | Y | 1.735 .9 | 868.4 | 1.718 .8 | 1.717 .9 | 15 |
| 13 | 1,758.6 | 879.8 | 1.741 .6 | 1,740.6 | D | 1,572.8 | 786.9 | 1,555.8 | 1.554.8 | 14 |
| 14 | 1.857 .7 | 929.4 | 1,840.7 | 1,839.7 | V | 1,457.8 | 729.4 | 1,440.8 | 1,439.8 | 13 |
| 15 | 1,986.7 | 993.9 | 1,969.7 | 1,968.7 | E | 1.358 .7 | 679.9 | 1,341.7 | 1,340.7 | 12 |
| 16 | 2,100.8 | 1.050.9 | 2,083.8 | 2,082.8 | N | 1,229.7 | 615.3 | 1.212 .6 | 1.211 .7 | 11 |
| 17 | 2,256.9 | 1.128.9 | 2,239.9 | 2,238.9 | R | 1.115.6 | 558.3 | 1,098.6 | 1.097 .6 | 10 |
| 18 | 2,353.9 | 1.177 .5 | 2,336.9 | 2,335.9 | P | 959.5 | 480.3 | 942.5 | 941.5 | 9 |
| 19 | 2,411.0 | 1,206.0 | 2,393.9 | 2,392.9 | G | 862.5 | 431.7 | 845.5 | 844.5 | 8 |
| 20 | 2,558.0 | 1.279.5 | 2,541.0 | 2,540.0 | F | 805.5 | 403.2 | 788.4 | 787.4 | 7 |
| 21 | 2,629.1 | 1,315.0 | 2,612.0 | 2,611.0 | A | 658.4 | 329.7 | 641.4 | 640.4 | 6 |
| 22 | 2,700.1 | 1,350.6 | 2,683.1 | 2,682.1 | A | 587.4 |  | 570.3 | 569.3 | 5 |
| 23 | $2,799.2$ | 1.400.1 | 2,782.1 | 2.781 .2 | V | 516.3 |  | 499.3 | 498.3 | 4 |
| 24 | 2,928.2 | 1.464.6 | 2,911.2 | $2,910.2$ | E | 417.2 |  | 400.2 | 399.2 | 3 |
| 25 | 3,041.3 | 1,521.1 | 3,024.3 | 3,023.3 | L | 288.2 |  | 271.2 |  | 2 |
| 26 | 3,215.4 | 1,608.2 | 3,198.4 | 3,197.4 | R | 175.1 |  | 158.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp <br> M.W. | Charge | Delta | Mascot lon score |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| (R)EyVKQTWNLQGQALEQAIISQKPQLEK(L) | pY | 1084.2190 | 3249.635 | 3 | -0.009 | 66.8 |



| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | $Y$ Ions | $Y+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 130.0 |  |  | 112.0 | E | 3,250.7 | 1.625 .8 | 3,233.6 | 3,232.6 | 27 |
| 2 | 373.1 |  |  | 355.1 | Y+80 | 3,121.6 | 1,561.3 | 3,104.6 | 3,103.6 | 26 |
| 3 | 472.1 |  |  | 454.1 | V | 2,878.6 | 1.439.8 | 2,861.6 | 2,860.6 | 25 |
| 4 | 600.2 | 300.6 | 583.2 | 582.2 | K | 2,779.5 | 1.390 .3 | 2,762.5 | 2,761.5 | 24 |
| 5 | 728.3 | 364.7 | 711.3 | 710.3 | Q | 2,651.4 | 1.326.2 | 2,634.4 | 2,633.4 | 3 |
| 6 | 829.3 | 415.2 | 812.3 | 811.3 | T | 2,523.4 | 1.262.2 | 2.506 .3 | 2,505.3 | 22 |
| 7 | 1,015.4 | 508.2 | 998.4 | 997.4 | w | 2,422.3 | 1.211.7 | 2,405.3 | 2.404 .3 | 21 |
| 8 | 1.129.5 | 565.2 | 1,112.4 | 1.111.5 | N | 2,236.2 | 1.118.6 | 2,219.2 | 2,218.2 | 20 |
| 9 | 1.242.6 | 621.8 | 1,225.5 | 1.224.5 | L | 2,122.2 | 1.061 .6 | 2,105.2 | 2,104.2 | 19 |
| 10 | 1.370.6 | 685.8 | 1,353.6 | 1.352.6 | Q | 2,009.1 | 1.005.1 | 1,992.1 | 1,991.1 | 18 |
| 11 | 1.427.6 | 714.3 | 1.410 .6 | 1,409.6 | G | 1.881 .0 | 941.0 | 1,864.0 | 1,863.0 | 17 |
| 12 | 1.555.7 | 778.4 | 1,538.7 | 1.537 .7 | Q | 1,824.0 | 912.5 | 1,807.0 | 1,806.0 | 16 |
| 13 | 1,626.7 | 813.9 | 1,609.7 | 1.608.7 | A | 1.696 .0 | 848.5 | 1.678 .9 | 1,678.0 | 15 |
| 14 | 1,739.8 | 870.4 | 1,722.8 | 1.721 .8 | L | 1,624.9 | 813.0 | 1,607.9 | 1,606.9 | 14 |
| 15 | 1.868.9 | 934.9 | 1.851 .8 | 1,850.8 | E | 1.511 .8 | 756.4 | 1,494.8 | 1,493.8 | 13 |
| 16 | 1.996.9 | 999.0 | 1,979.9 | 1.978 .9 | Q | 1.382 .8 | 691.9 | 1,365.8 | 1.364 .8 | 12 |
| 17 | 2.068 .0 | 1,034.5 | 2.050 .9 | 2,049.9 | A | 1.254 .7 | 627.9 | 1,237.7 | 1.236.7 | 11 |
| 18 | 2,181.0 | 1.091.0 | 2,164.0 | 2,163.0 | I | 1.183.7 | 592.4 | 1,166.7 | 1,165.7 | 10 |
| 19 | 2,294.1 | 1.147.6 | 2,277.1 | 2,276.1 | I | 1.070.6 | 535.8 | 1,053.6 | 1.052.6 | 9 |
| 20 | 2,381.2 | 1,191.1 | 2,364.1 | 2,363.1 | 5 | 957.5 | 479.3 | 940.5 | 939.5 | 8 |
| 21 | 2,509.2 | 1,255.1 | 2,492.2 | 2,491.2 | Q | 870.5 | 435.8 | 853.5 | 852.5 | 7 |
| 22 | 2,637.3 | 1.319.2 | 2,620.3 | 2,619.3 | K | 742.4 | 371.7 | 725.4 | 724.4 | 6 |
| 23 | 2,734.4 | 1.367 .7 | 2,717.3 | 2.716 .3 | P | 614.4 |  | 597.3 | 596.3 | 5 |
| 24 | 2,862.4 | 1.431.7 | 2,845.4 | 2,844.4 | Q | 517.3 |  | 500.3 | 499.3 | 4 |
| 25 | 2,975.5 | 1.488.3 | 2.958 .5 | 2.957 .5 | L | 389.2 |  | 372.2 | 371.2 | 3 |
| 26 | 3,104.5 | 1.552.8 | 3,087.5 | 3,086.5 | E | 276.2 |  | 259.1 | 258.1 | 2 |
| 27 | 3,250.7 | 1.625.8 | 3,233.6 | 3,232.6 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp <br> M.W. | Charge | Delta | Mascot lon score |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $($ K)LLTLEDKELGSGNFGtVK(K) | pT | 667.6685 | 1999.984 | 3 | -0.003 | 43.6 |



| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | $Y$ Ions | $Y+2 \mathrm{H}$ | Y-NH3 | Y-H2O | $Y$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 114.1 |  |  |  | L | 2,001.0 | 1,001.0 | 1,984.0 | 1.983 .0 | 18 |
| 2 | 227.2 |  |  |  | L | 1,887.9 | 944.5 | 1,870.9 | 1,869.9 | 17 |
| 3 | 328.2 |  |  | 310.2 | T | 1,774.8 | 887.9 | 1.757 .8 | 1.756 .8 | 16 |
| 4 | 441.3 |  |  | 423.3 | L | 1.673 .8 | 837.4 | 1,656.8 | $1,655.8$ | 15 |
| 5 | 570.3 |  |  | 552.3 | E | 1,560.7 | 780.9 | 1,543.7 | 1,542.7 | 14 |
| 6 | 685.4 | 343.2 |  | 667.4 | D | 1,431.7 | 716.3 | 1,414.6 | 1,413.6 | 13 |
| 7 | 813.5 | 407.2 | 796.4 | 795.5 | K | 1,316.6 | 658.8 | 1.299.6 | 1,298.6 | 12 |
| 8 | 942.5 | 471.8 | 925.5 | 924.5 | E | 1,188.5 | 594.8 | 1,171.5 | 1,170.5 | 11 |
| 9 | 1.055 .6 | 528.3 | 1,038.6 | 1,037.6 | L | 1.059.5 | 530.2 | 1,042.5 | 1,041.5 | 10 |
| 10 | 1.112.6 | 556.8 | 1,095.6 | 1.094 .6 | G | 946.4 | 473.7 | 929.4 | 928.4 | 9 |
| 11 | 1,199.7 | 600.3 | 1,182.6 | 1.181 .6 | 5 | 889.4 | 445.2 | 872.4 | 871.4 | 8 |
| 12 | 1,256.7 | 628.8 | 1,239.6 | 1,238.7 | G | 802.3 | 401.7 | 785.3 | 784.3 | 7 |
| 13 | 1,370.7 | 685.9 | 1,353.7 | 1,352.7 | N | 745.3 | 373.2 | 728.3 | 727.3 | 6 |
| 14 | 1.517 .8 | 759.4 | 1,500.8 | 1,499.8 | F | 631.3 |  | 614.3 | 613.3 | 5 |
| 15 | 1,574.8 | 787.9 | 1,557.8 | 1.556 .8 | G | 484.2 |  | 467.2 | 466.2 | 4 |
| 16 | 1.755 .8 | 878.4 | 1.738 .8 | 1,737.8 | T+80 | 427.2 |  | 410.2 | 409.2 | 3 |
| 17 | 1,854.9 | 927.9 | 1,837.9 | 1,836.9 | V | 246.2 |  | 229.2 |  | 2 |
| 18 | 2,001.0 | 1.001.0 | 1,984.0 | 1,983.0 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp <br> M.W. | Charge | Delta | Mascot lon score |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| (R)QESTVSFNPyEPELAPWAADKGPQR(E) | pY | 966.4413 | 2896.302 | 3 | -0.005 | 62.7 |



| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B- $\mathrm{H}_{2} \mathrm{O}$ | AA | $Y$ Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 129.1 |  | 112.0 |  | Q | 2,897.3 | 1,449.2 | 2.880 .3 | 2.879 .3 | 25 |
| 2 | 258.1 |  | 241.1 | 240.1 | E | $2,769.3$ | 1.385 .1 | 2.752 .2 | 2.751 .2 | 24 |
| 3 | 345.1 |  | 328.1 | 327.1 | 5 | 2,640.2 | 1.320 .6 | 2.623 .2 | 2.622 .2 | 23 |
| 4 | 446.2 |  | 429.2 | 428.2 | T | 2,553.2 | 1.277 .1 | 2.536 .2 | 2,535.2 | 22 |
| 5 | 545.3 |  | 528.2 | 527.2 | V | 2,452.1 | 1.226.6 | 2,435.1 | 2,434.1 | 21 |
| 6 | 632.3 | 316.6 | 615.3 | 614.3 | 5 | 2,353.1 | 1.177 .0 | 2,336.0 | 2,335.1 | 20 |
| 7 | 779.4 | 390.2 | 762.3 | 761.3 | F | 2,266.0 | 1.133 .5 | 2,249.0 | 2.248 .0 | 19 |
| 8 | 893.4 | 447.2 | 876.4 | 875.4 | N | 2.119 .0 | 1.060.0 | 2,101.9 | 2.101 .0 | 18 |
| 9 | 990.5 | 495.7 | 973.4 | 972.4 | P | 2,004.9 | 1.003 .0 | 1.987 .9 | 1,986.9 | 17 |
| 10 | 1.233.5 | 617.2 | 1,216.5 | 1.215.5 | $\mathrm{Y}+80$ | 1,907.9 | 954.4 | 1.890 .8 | 1.889 .9 | 16 |
| 11 | 1.362 .5 | 681.8 | 1,345.5 | 1,344.5 | E | 1.664.8 | 832.9 | 1.647 .8 | 1.646 .8 | 15 |
| 12 | 1.459.6 | 730.3 | 1,442.6 | 1,441.6 | P | 1.535 .8 | 768.4 | 1.518.8 | 1.517 .8 | 14 |
| 13 | 1,588.6 | 794.8 | 1.571.6 | 1.570 .6 | E | 1.438.7 | 719.9 | 1.421.7 | 1,420.7 | 13 |
| 14 | 1.701 .7 | 851.4 | 1,684.7 | 1.683.7 | L | 1.309 .7 | 655.4 | 1,292.7 | 1,291.7 | 12 |
| 15 | 1.772 .7 | 886.9 | 1,755.7 | 1.754.7 | A | 1.196.6 | 598.8 | 1.179 .6 | 1.178 .6 | 11 |
| 16 | 1,869.8 | 935.4 | 1.852 .8 | 1,851.8 | P | 1.125.6 | 563.3 | 1,108.6 | 1.107 .6 | 10 |
| 17 | 2.055 .9 | 1,028.4 | $2,038.8$ | 2,037.9 | W | 1.028.5 | 514.8 | 1,011.5 | 1.010.5 | 9 |
| 18 | 2,126.9 | 1,064.0 | 2.109 .9 | 2,108.9 | A | 842.4 | 421.7 | 825.4 | 824.4 | 8 |
| 19 | 2.197 .9 | 1.099 .5 | 2,180.9 | 2.179 .9 | A | 771.4 | 386.2 | 754.4 | 753.4 | 7 |
| 20 | 2,313.0 | 1.157 .0 | 2,295.9 | 2,295.0 | D | 700.4 | 350.7 | 683.3 | 682.4 | 6 |
| 21 | 2.441 .1 | 1.221.0 | 2,424.0 | 2,423.1 | K | 585.3 | 293.2 | 568.3 |  | 5 |
| 22 | 2,498.1 | 1.249 .5 | 2,481.1 | 2,480.1 | G | 457.3 |  | 440.2 |  | 4 |
| 23 | 2.595 .1 | 1,298.1 | 2,578.1 | 2,577.1 | P | 400.2 |  | 383.2 |  | 3 |
| 24 | 2.723 .2 | 1.362.1 | 2.706 .2 | 2,705.2 | Q | 303.2 |  | 286.2 |  | 2 |
| 25 | 2.897 .3 | 1,449.2 | 2.880 .3 | 2,879.3 | R | 175.1 |  | 158.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp <br> M.W. | Charge | Delta | Mascot lon score |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| $($ K)sYSFPKPGHR(K) | pS | 628.2836 | 1254.553 | 2 | -0.002 | 30.2 |



| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B H 2 O | AA | $Y$ Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 168.0 |  |  | 150.0 | S+80 | 1,255.6 | 628.3 | 1,238.5 | 1,237.6 | 10 |
| 2 | 331.1 |  |  | 313.1 | Y | 1,088.6 | 544.8 | 1,071.5 | 1,070.6 | 9 |
| 3 | 418.1 |  |  | 400.1 | 5 | 925.5 | 463.3 | 908.5 | 907.5 | 8 |
| 4 | 565.2 |  |  | 547.2 | F | 838.5 | 419.7 | 821.4 |  | 7 |
| 5 | 662.2 |  |  | 644.2 | P | 691.4 | 346.2 | 674.4 |  | 6 |
| 6 | 790.3 | 395.7 | 773.3 | 772.3 | K | 594.3 | 297.7 | 577.3 |  | 5 |
| 7 | 887.4 | 444.2 | 870.3 | 869.4 | P | 466.3 | 233.6 | 449.2 |  | 4 |
| 8 | 944.4 | 472.7 | 927.4 | 926.4 | G | 369.2 | 185.1 | 352.2 |  | 3 |
| 9 | 1.081.5 | 541.2 | 1,064.4 | 1.063.4 | H | 312.2 | 156.6 | 295.2 |  | 2 |
| 10 | 1,255.6 | 628.3 | 1,238.5 | 1,237.6 | R | 175.1 |  | 158.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| ADENYYK | pY | 491.6798 | 981.345 | 2 | 981.3481 | -0.003 | 17.4 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 72.0 |  |  |  | A | 982.4 | 491.7 | 965.3 | 964.3 | 7 |
| 2 | 187.1 |  |  | 169.1 | D | 911.3 | 456.2 | 894.3 | 893.3 | 6 |
| 3 | 316.1 |  |  | 298.1 | E | 796.3 |  | 779.3 | 778.3 | 5 |
| 4 | 430.2 |  | 413.1 | 412.1 | N | 667.2 |  | 650.2 |  | 4 |
| 5 | 593.2 |  | 576.2 | 575.2 | $Y$ | 553.2 |  | 536.2 |  | 3 |
| 6 | 836.2 | 418.6 | 819.2 | 818.2 | Y+80 | 390.1 |  | 373.1 |  | 2 |
| 7 | 982.4 | 491.7 | 965.3 | 964.3 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ADENYYK | pY | 491.6812 | 981.3478 | 2 | 981.3481 | -0.0002 | 38.99 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 72.0 |  |  |  | A | 982.4 | 491.7 | 965.3 | 964.3 | 7 |
| 2 | 187.1 |  |  | 169.1 | D | 911.3 | 456.2 | 894.3 | 893.3 | 6 |
| 3 | 316.1 |  |  | 298.1 | E | 796.3 |  | 779.3 | 778.3 | 5 |
| 4 | 430.2 |  | 413.1 | 412.1 | N | 667.2 |  | 650.2 |  | 4 |
| 5 | 673.2 |  | 656.2 | 655.2 | Y+80 | 553.2 |  | 536.2 |  | 3 |
| 6 | 836.2 | 418.6 | 819.2 | 818.2 | $Y$ | 310.2 |  | 293.1 |  | 2 |
| 7 | 982.4 | 491.7 | 965.3 | 964.3 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| EVYLDRK | pY | 501.736 | 1001.4574 | 2 | 1001.4583 | -0.0008 | 26.19 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 130.0 |  |  | 112.0 | E | 1,002.5 | 501.7 | 985.4 | 984.5 | 7 |
| 2 | 229.1 |  |  | 211.1 | Y | 873.4 | 437.2 | 856.4 | 855.4 | 6 |
| 3 | 472.1 |  |  | 454.1 | Y+80 | 774.4 | 387.7 | 757.3 | 756.3 | 5 |
| 4 | 585.2 |  |  | 567.2 | L | 531.3 | 266.2 | 514.3 | 513.3 | 4 |
| 5 | 700.3 |  |  | 682.2 | D | 418.2 | 209.6 | 401.2 | 400.2 | 3 |
| 6 | 856.4 | 428.7 | 839.3 | 838.3 | R | 303.2 | 152.1 | 286.2 |  | 2 |
| 7 | 1,002.5 | 501.7 | 985.4 | 984.5 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| KGYYQMK | Mox; pY | 507.2101 | 1012.4056 | 2 | 1012.4089 | -0.0032 | 14.54 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AH | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 129.1 | 65.1 | 112.1 |  | K | 1,013.4 | 507.2 | 996.4 |  | 7 |
| 2 | 186.1 | 93.6 | 169.1 |  | G | 885.3 | 443.2 | 868.3 |  | 6 |
| 3 | 429.2 | 215.1 | 412.1 |  | Y+80 | 828.3 |  | 811.3 |  | 5 |
| 4 | 592.2 | 296.6 | 575.2 |  | Y | 585.3 |  | 568.2 |  | 4 |
| 5 | 720.3 | 360.6 | 703.2 |  | Q | 422.2 |  | 405.2 |  | 3 |
| 6 | 867.3 | 434.2 | 850.3 |  | M+16 | 294.1 |  | 277.1 |  | 2 |
| 7 | 1,013.4 | 507.2 | 996.4 |  | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| KSSPPAQGNR | pS | 512.7313 | 1023.448 | 2 | 1023.4498 | -0.0018 | 21.24 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 129.1 | 65.1 | 112.1 |  | K | 1,024.5 | 512.7 | 1,007.4 | 1,006.4 | 9 |
| 2 | 216.1 | 108.6 | 199.1 | 198.1 | S | 896.4 | 448.7 | 879.3 | 878.4 | 8 |
| 3 | 383.1 | 192.1 | 366.1 | 365.1 | S+80 | 809.3 | 405.2 | 792.3 | 791.3 | 7 |
| 4 | 480.2 | 240.6 | 463.2 | 462.2 | P | 642.3 | 321.7 | 625.3 |  | 6 |
| 5 | 551.2 | 276.1 | 534.2 | 533.2 | A | 545.3 |  | 528.3 |  | 5 |
| 6 | 679.3 | 340.1 | 662.3 | 661.3 | Q | 474.2 |  | 457.2 |  | 4 |
| 7 | 736.3 | 368.7 | 719.3 | 718.3 | G | 346.2 |  | 329.2 |  | 3 |
| 8 | 850.3 | 425.7 | 833.3 | 832.3 | N | 289.2 |  | 272.1 |  | 2 |
| 9 | 1,024.5 | 512.7 | 1,007.4 | 1,006.4 | R | 175.1 |  | 158.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| NyyyDVVN | pY | 565.2149 | 1128.4152 | 2 | 1128.4165 | -0.0012 | 10.88 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 115.1 |  | 98.0 |  | N | 1,129.4 |  | 1,112.4 | 1,111.4 | 8 |
| 2 | 278.1 |  | 261.1 |  | $Y$ | 1,015.4 |  | 998.4 | 997.4 | 7 |
| 3 | 441.2 |  | 424.2 |  | $Y$ | 852.3 |  | 835.3 | 834.3 | 6 |
| 4 | 684.2 |  | 667.2 |  | Y+80 | 689.3 |  | 672.2 | 671.2 | 5 |
| 5 | 799.2 |  | 782.2 | 781.2 | D | 446.2 |  | 429.2 | 428.2 | 4 |
| 6 | 898.3 | 449.7 | 881.3 | 880.3 | $Y$ | 331.2 |  | 314.2 |  | 3 |
| 7 | 997.4 | 499.2 | 980.3 | 979.4 | $Y$ | 232.1 |  | 215.1 |  | 2 |
| 8 | 1,129.4 | 565.2 | 1,112.4 | 1,111.4 | N | 133.1 |  | 116.0 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| SYSFPKPGHR | pS | 419.1918 | 1254.5536 | 3 | 1254.5547 | -0.0011 | 19.84 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 88.0 |  |  | 70.0 | S | 1,255.6 | 628.3 | 1,238.5 | 1,237.6 | 10 |
| 2 | 251.1 |  |  | 233.1 | $Y$ | 1,168.5 | 584.8 | 1,151.5 | 1,150.5 | 9 |
| 3 | 418.1 |  |  | 400.1 | S+80 | 1,005.5 | 503.2 | 988.4 | 987.5 | 8 |
| 4 | 565.2 |  |  | 547.2 | F | 838.5 | 419.7 | 821.4 |  | 7 |
| 5 | 662.2 |  |  | 644.2 | P | 691.4 | 346.2 | 674.4 |  | 6 |
| 6 | 790.3 | 395.7 | 773.3 | 772.3 | K | 594.3 | 297.7 | 577.3 |  | 5 |
| 7 | 887.4 | 444.2 | 870.3 | 869.4 | P | 466.3 | 233.6 | 449.2 |  | 4 |
| 8 | 944.4 | 472.7 | 927.4 | 926.4 | G | 369.2 | 185.1 | 352.2 |  | 3 |
| 9 | 1,081.5 | 541.2 | 1,064.4 | 1,063.4 | H | 312.2 | 156.6 | 295.2 |  | 2 |
| 10 | 1,255.6 | 628.3 | 1,238.5 | 1,237.6 | R | 175.1 |  | 158.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| SYSFPKPGHR | pY | 419.1927 | 1254.5563 | 3 | 1254.5547 | 0.0016 | 33.78 |



| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 88.0 |  |  | 70.0 | S | 1,255.6 | 628.3 | 1,238.5 | 1,237.6 | 10 |
| 2 | 331.1 |  |  | 313.1 | Y+80 | 1,168.5 | 584.8 | 1,151.5 | 1,150.5 | 9 |
| 3 | 418.1 |  |  | 400.1 | S | 925.5 | 463.3 | 908.5 | 907.5 | 8 |
| 4 | 565.2 |  |  | 547.2 | F | 838.5 | 419.7 | 821.4 |  | 7 |
| 5 | 662.2 |  |  | 644.2 | P | 691.4 | 346.2 | 674.4 |  | 6 |
| 6 | 790.3 | 395.7 | 773.3 | 772.3 | K | 594.3 | 297.7 | 577.3 |  | 5 |
| 7 | 887.4 | 444.2 | 870.3 | 869.4 | P | 466.3 | 233.6 | 449.2 |  | 4 |
| 8 | 944.4 | 472.7 | 927.4 | 926.4 | G | 369.2 | 185.1 | 352.2 |  | 3 |
| 9 | 1,081.5 | 541.2 | 1,064.4 | 1,063.4 | H | 312.2 | 156.6 | 295.2 |  | 2 |
| 10 | 1,255.6 | 628.3 | 1,238.5 | 1,237.6 | R | 175.1 |  | 158.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ALRADENYYK | pY | 661.7919 | 1321.5692 | 2 | 1321.5703 | -0.0011 | 21.5 |



| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 72.0 |  |  |  | A | 1,322.6 | 661.8 | 1,305.6 | 1,304.6 | 10 |
| 2 | 185.1 |  |  |  | L | 1,251.5 | 626.3 | 1,234.5 | 1,233.5 | 9 |
| 3 | 341.2 | 171.1 | 324.2 |  | R | 1,138.5 | 569.7 | 1,121.4 | 1,120.4 | 8 |
| 4 | 412.3 | 206.6 | 395.2 |  | A | 982.4 | 491.7 | 965.3 | 964.3 | 7 |
| 5 | 527.3 | 264.2 | 510.3 | 509.3 | D | 911.3 | 456.2 | 894.3 | 893.3 | 6 |
| 6 | 656.3 | 328.7 | 639.3 | 638.3 | E | 796.3 |  | 779.3 | 778.3 | 5 |
| 7 | 770.4 | 385.7 | 753.4 | 752.4 | N | 667.2 |  | 650.2 |  | 4 |
| 8 | 933.4 | 467.2 | 916.4 | 915.4 | $Y$ | 553.2 |  | 536.2 |  | 3 |
| 9 | 1,176.5 | 588.7 | 1,159.4 | 1,158.5 | Y+80 | 390.1 |  | 373.1 |  | 2 |
| 10 | 1,322.6 | 661.8 | 1,305.6 | 1,304.6 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ALRADENYYK | pY | 661.7921 | 1321.5696 | 2 | 1321.5703 | -0.0007 | 30.3 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 72.0 |  |  |  | A | 1,322.6 | 661.8 | 1,305.6 | 1,304.6 | 10 |
| 2 | 185.1 |  |  |  | L | 1,251.5 | 626.3 | 1,234.5 | 1,233.5 | 9 |
| 3 | 341.2 | 171.1 | 324.2 |  | R | 1,138.5 | 569.7 | 1,121.4 | 1,120.4 | 8 |
| 4 | 412.3 | 206.6 | 395.2 |  | A | 982.4 | 491.7 | 965.3 | 964.3 | 7 |
| 5 | 527.3 | 264.2 | 510.3 | 509.3 | D | 911.3 | 456.2 | 894.3 | 893.3 | 6 |
| 6 | 656.3 | 328.7 | 639.3 | 638.3 | E | 796.3 |  | 779.3 | 778.3 | 5 |
| 7 | 770.4 | 385.7 | 753.4 | 752.4 | N | 667.2 |  | 650.2 |  | 4 |
| 8 | 1,013.4 | 507.2 | 996.4 | 995.4 | Y+80 | 553.2 |  | 536.2 |  | 3 |
| 9 | 1,176.5 | 588.7 | 1,159.4 | 1,158.5 | $Y$ | 310.2 |  | 293.1 |  | 2 |
| 10 | 1,322.6 | 661.8 | 1,305.6 | 1,304.6 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| NVLLVTQHYAK | pY | 683.3502 | 1364.6858 | 2 | 1364.6853 | 0.0005 | 33.17 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 115.1 |  | 98.0 |  | N | 1,365.7 | 683.3 | 1,348.7 | 1,347.7 | 11 |
| 2 | 214.1 |  | 197.1 |  | Y | 1,251.6 | 626.3 | 1,234.6 | 1,233.6 | 10 |
| 3 | 327.2 |  | 310.2 |  | L | 1,152.6 | 576.8 | 1,135.6 | 1,134.6 | 9 |
| 4 | 440.3 |  | 423.3 |  | L | 1,039.5 | 520.3 | 1,022.5 | 1,021.5 | 8 |
| 5 | 539.4 |  | 522.3 |  | V | 926.4 | 463.7 | 909.4 | 908.4 | 7 |
| 6 | 640.4 | 320.7 | 623.4 | 622.4 | T | 827.3 | 414.2 | 810.3 | 809.3 | 6 |
| 7 | 768.5 | 384.7 | 751.4 | 750.5 | Q | 726.3 | 363.7 | 709.3 |  | 5 |
| 8 | 905.5 | 453.3 | 888.5 | 887.5 | H | 598.2 | 299.6 | 581.2 |  | 4 |
| 9 | 1,148.5 | 574.8 | 1,131.5 | 1,130.5 | Y+80 | 461.2 |  | 444.2 |  | 3 |
| 10 | 1,219.6 | 610.3 | 1,202.6 | 1,201.6 | A | 218.1 |  | 201.1 |  | 2 |
| 11 | 1,365.7 | 683.3 | 1,348.7 | 1,347.7 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\underline{\text { YLEESNFVHR }}$ | pY | 687.2959 | 1372.5772 | 2 | 1372.5813 | -0.004 | 18.66 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 244.0 |  |  |  | Y+80 | 1,373.6 | 687.3 | 1,356.6 | 1,355.6 | 10 |
| 2 | 357.1 |  |  |  | L | 1,130.6 | 565.8 | 1,113.5 | 1,112.5 | 9 |
| 3 | 486.2 |  |  | 468.2 | E | 1,017.5 | 509.2 | 1,000.4 | 999.5 | 8 |
| 4 | 615.2 |  |  | 597.2 | E | 888.4 | 444.7 | 871.4 | 870.4 | 7 |
| 5 | 702.2 |  |  | 684.2 | S | 759.4 | 380.2 | 742.4 | 741.4 | 6 |
| 6 | 816.3 | 408.6 | 799.3 | 798.3 | N | 672.4 | 336.7 | 655.3 |  | 5 |
| 7 | 963.3 | 482.2 | 946.3 | 945.3 | F | 558.3 | 279.7 | 541.3 |  | 4 |
| 8 | 1,062.4 | 531.7 | 1,045.4 | 1,044.4 | $Y$ | 411.2 | 206.1 | 394.2 |  | 3 |
| 9 | 1,199.5 | 600.2 | 1,182.5 | 1,181.5 | H | 312.2 | 156.6 | 295.2 |  | 2 |
| 10 | 1,373.6 | 687.3 | 1,356.6 | 1,355.6 | R | 175.1 |  | 158.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| LRNYYYDVVN | pY | 699.8079 | 1397.6012 | 2 | Score |  |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 114.1 |  |  |  | L | 1,398.6 | 699.8 | 1,381.6 | 1,380.6 | 10 |
| 2 | 270.2 | 135.6 | 253.2 |  | R | 1,285.5 | 643.3 | 1,268.5 | 1,267.5 | 9 |
| 3 | 384.2 | 192.6 | 367.2 |  | N | 1,129.4 |  | 1,112.4 | 1,111.4 | 8 |
| 4 | 547.3 | 274.2 | 530.3 |  | $Y$ | 1,015.4 |  | 998.4 | 997.4 | 7 |
| 5 | 790.3 | 395.7 | 773.3 |  | Y+80 | 852.3 |  | 835.3 | 834.3 | 6 |
| 6 | 953.4 | 477.2 | 936.4 |  | $Y$ | 609.3 |  | 592.3 | 591.3 | 5 |
| 7 | 1,068.4 | 534.7 | 1,051.4 | 1,050.4 | D | 446.2 |  | 429.2 | 428.2 | 4 |
| 8 | 1,167.5 | 584.2 | 1,150.5 | 1,149.5 | Y | 331.2 |  | 314.2 |  | 3 |
| 9 | 1,266.6 | 633.8 | 1,249.5 | 1,248.5 | Y | 232.1 |  | 215.1 |  | 2 |
| 10 | 1,398.6 | 699.8 | 1,381.6 | 1,380.6 | N | 133.1 |  | 116.0 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| LRNYYYDVVN | 2 pY | 739.7906 | 1477.5666 | 2 | 1477.568 | -0.0013 | 10.17 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 114.1 |  |  |  | L | 1,478.6 | 739.8 | 1,461.5 | 1,460.6 | 10 |
| 2 | 270.2 | 135.6 | 253.2 |  | R | 1,365.5 | 683.2 | 1,348.5 | 1,347.5 | 9 |
| 3 | 384.2 | 192.6 | 367.2 |  | N | 1,209.4 |  | 1,192.4 | 1,191.4 | 8 |
| 4 | 547.3 | 274.2 | 530.3 |  | $Y$ | 1,095.3 |  | 1,078.3 | 1,077.3 | 7 |
| 5 | 790.3 | 395.7 | 773.3 |  | Y+80 | 932.3 |  | 915.3 | 914.3 | 6 |
| 6 | 1,033.4 | 517.2 | 1,016.3 |  | Y+80 | 689.3 |  | 672.2 | 671.2 | 5 |
| 7 | 1,148.4 | 574.7 | 1,131.4 | 1,130.4 | D | 446.2 |  | 429.2 | 428.2 | 4 |
| 8 | 1,247.5 | 624.2 | 1,230.4 | 1,229.4 | Y | 331.2 |  | 314.2 |  | 3 |
| 9 | 1,346.5 | 673.8 | 1,329.5 | 1,328.5 | Y | 232.1 |  | 215.1 |  | 2 |
| 10 | 1,478.6 | 739.8 | 1,461.5 | 1,460.6 | N | 133.1 |  | 116.0 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| LRNYYYDVVN | 2 pY | 739.7911 | 1477.5676 | 2 | 1477.568 | -0.0003 | 21.12 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 114.1 |  |  |  | L | 1,478.6 | 739.8 | 1,461.5 | 1,460.6 | 10 |
| 2 | 270.2 | 135.6 | 253.2 |  | R | 1,365.5 | 683.2 | 1,348.5 | 1,347.5 | 9 |
| 3 | 384.2 | 192.6 | 367.2 |  | N | 1,209.4 |  | 1,192.4 | 1,191.4 | 8 |
| 4 | 627.3 | 314.1 | 610.2 |  | Y+80 | 1,095.3 |  | 1,078.3 | 1,077.3 | 7 |
| 5 | 790.3 | 395.7 | 773.3 |  | $Y$ | 852.3 |  | 835.3 | 834.3 | 6 |
| 6 | 1,033.4 | 517.2 | 1,016.3 |  | Y+80 | 689.3 |  | 672.2 | 671.2 | 5 |
| 7 | 1,148.4 | 574.7 | 1,131.4 | 1,130.4 | D | 446.2 |  | 429.2 | 428.2 | 4 |
| 8 | 1,247.5 | 624.2 | 1,230.4 | 1,229.4 | Y | 331.2 |  | 314.2 |  | 3 |
| 9 | 1,346.5 | 673.8 | 1,329.5 | 1,328.5 | V | 232.1 |  | 215.1 |  | 2 |
| 10 | 1,478.6 | 739.8 | 1,461.5 | 1,460.6 | N | 133.1 |  | 116.0 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| IKSYSFPKPGGR | pS | 499.5849 | 1495.7329 | 3 | 1495.7337 | -0.0008 | 31.6 |



| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 114.1 |  |  |  | I | 1,496.7 | 748.9 | 1,479.7 | 1,478.7 | 12 |
| 2 | 242.2 | 121.6 | 225.2 |  | K | 1,383.7 | 692.3 | 1,366.6 | 1,365.6 | 11 |
| 3 | 409.2 | 205.1 | 392.2 | 391.2 | S+80 | 1,255.6 | 628.3 | 1,238.5 | 1,237.6 | 10 |
| 4 | 572.2 | 286.6 | 555.2 | 554.2 | Y | 1,088.6 | 544.8 | 1,071.5 | 1,070.6 | 9 |
| 5 | 659.3 | 330.1 | 642.3 | 641.3 | S | 925.5 | 463.3 | 908.5 | 907.5 | 8 |
| 6 | 806.3 | 403.7 | 789.3 | 788.3 | F | 838.5 | 419.7 | 821.4 |  | 7 |
| 7 | 903.4 | 452.2 | 886.4 | 885.4 | P | 691.4 | 346.2 | 674.4 |  | 6 |
| 8 | 1,031.5 | 516.3 | 1,014.5 | 1,013.5 | K | 594.3 | 297.7 | 577.3 |  | 5 |
| 9 | 1,128.5 | 564.8 | 1,111.5 | 1,110.5 | P | 466.3 | 233.6 | 449.2 |  | 4 |
| 10 | 1,185.6 | 593.3 | 1,168.5 | 1,167.6 | G | 369.2 | 185.1 | 352.2 |  | 3 |
| 11 | 1,322.6 | 661.8 | 1,305.6 | 1,304.6 | H | 312.2 | 156.6 | 295.2 |  | 2 |
| 12 | 1,496.7 | 748.9 | 1,479.7 | 1,478.7 | R | 175.1 |  | 158.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| IKSYSFPKPGHR | pY | 499.5853 | 1495.7341 | 3 | 1495.7337 | 0.0004 | 23.85 |



| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 114.1 |  |  |  | I | 1,496.7 | 748.9 | 1,479.7 | 1,478.7 | 12 |
| 2 | 242.2 | 121.6 | 225.2 |  | K | 1,383.7 | 692.3 | 1,366.6 | 1,365.6 | 11 |
| 3 | 329.2 | 165.1 | 312.2 | 311.2 | S | 1,255.6 | 628.3 | 1,238.5 | 1,237.6 | 10 |
| 4 | 572.2 | 286.6 | 555.2 | 554.2 | Y+80 | 1,168.5 | 584.8 | 1,151.5 | 1,150.5 | 9 |
| 5 | 659.3 | 330.1 | 642.3 | 641.3 | S | 925.5 | 463.3 | 908.5 | 907.5 | 8 |
| 6 | 806.3 | 403.7 | 789.3 | 788.3 | F | 838.5 | 419.7 | 821.4 |  | 7 |
| 7 | 903.4 | 452.2 | 886.4 | 885.4 | P | 691.4 | 346.2 | 674.4 |  | 6 |
| 8 | 1,031.5 | 516.3 | 1,014.5 | 1,013.5 | K | 594.3 | 297.7 | 577.3 |  | 5 |
| 9 | 1,128.5 | 564.8 | 1,111.5 | 1,110.5 | P | 466.3 | 233.6 | 449.2 |  | 4 |
| 10 | 1,185.6 | 593.3 | 1,168.5 | 1,167.6 | G | 369.2 | 185.1 | 352.2 |  | 3 |
| 11 | 1,322.6 | 661.8 | 1,305.6 | 1,304.6 | H | 312.2 | 156.6 | 295.2 |  | 2 |
| 12 | 1,496.7 | 748.9 | 1,479.7 | 1,478.7 | R | 175.1 |  | 158.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| IKSYSFPKPGHR | pS | 499.5853 | 1495.7341 | 3 | 1495.7337 | 0.0004 | 30.79 |



| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 114.1 |  |  |  | I | 1,496.7 | 748.9 | 1,479.7 | 1,478.7 | 12 |
| 2 | 242.2 | 121.6 | 225.2 |  | K | 1,383.7 | 692.3 | 1,366.6 | 1,365.6 | 11 |
| 3 | 329.2 | 165.1 | 312.2 | 311.2 | S | 1,255.6 | 628.3 | 1,238.5 | 1,237.6 | 10 |
| 4 | 492.3 | 246.6 | 475.3 | 474.3 | $Y$ | 1,168.5 | 584.8 | 1,151.5 | 1,150.5 | 9 |
| 5 | 659.3 | 330.1 | 642.3 | 641.3 | S+80 | 1,005.5 | 503.2 | 988.4 | 987.5 | 8 |
| 6 | 806.3 | 403.7 | 789.3 | 788.3 | F | 838.5 | 419.7 | 821.4 |  | 7 |
| 7 | 903.4 | 452.2 | 886.4 | 885.4 | P | 691.4 | 346.2 | 674.4 |  | 6 |
| 8 | 1,031.5 | 516.3 | 1,014.5 | 1,013.5 | K | 594.3 | 297.7 | 577.3 |  | 5 |
| 9 | 1,128.5 | 564.8 | 1,111.5 | 1,110.5 | P | 466.3 | 233.6 | 449.2 |  | 4 |
| 10 | 1,185.6 | 593.3 | 1,168.5 | 1,167.6 | G | 369.2 | 185.1 | 352.2 |  | 3 |
| 11 | 1,322.6 | 661.8 | 1,305.6 | 1,304.6 | H | 312.2 | 156.6 | 295.2 |  | 2 |
| 12 | 1,496.7 | 748.9 | 1,479.7 | 1,478.7 | R | 175.1 |  | 158.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| NYLGGFALSVAHGR | pY | 771.3672 | 1540.7198 | 2 | 1540.7188 | 0.0011 | 39.23 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 115.1 |  | 98.0 |  | N | 1,541.7 | 771.4 | 1,524.7 | 1,523.7 | 14 |
| 2 | 358.1 |  | 341.1 |  | Y+80 | 1,427.7 | 714.3 | 1,410.7 | 1,409.7 | 13 |
| 3 | 471.2 |  | 454.1 |  | L | 1,184.7 | 592.8 | 1,167.6 | 1,166.6 | 12 |
| 4 | 528.2 |  | 511.2 |  | G | 1,071.6 | 536.3 | 1,054.5 | 1,053.6 | 11 |
| 5 | 585.2 |  | 568.2 |  | G | 1,014.5 | 507.8 | 997.5 | 996.5 | 10 |
| 6 | 732.3 | 366.6 | 715.2 |  | F | 957.5 | 479.3 | 940.5 | 939.5 | 9 |
| 7 | 803.3 | 402.2 | 786.3 |  | A | 810.5 | 405.7 | 793.4 | 792.4 | 8 |
| 8 | 916.4 | 458.7 | 899.4 |  | L | 739.4 | 370.2 | 722.4 | 721.4 | 7 |
| 9 | 1,003.4 | 502.2 | 986.4 | 985.4 | S | 626.3 | 313.7 | 609.3 | 608.3 | 6 |
| 10 | 1,102.5 | 551.8 | 1,085.5 | 1,084.5 | 7 | 539.3 | 270.2 | 522.3 |  | 5 |
| 11 | 1,173.5 | 587.3 | 1,156.5 | 1,155.5 | A | 440.2 | 220.6 | 423.2 |  | 4 |
| 12 | 1,310.6 | 655.8 | 1,293.6 | 1,292.6 | H | 369.2 | 185.1 | 352.2 |  | 3 |
| 13 | 1,367.6 | 684.3 | 1,350.6 | 1,349.6 | G | 232.1 |  | 215.1 |  | 2 |
| 14 | 1,541.7 | 771.4 | 1,524.7 | 1,523.7 | R | 175.1 |  | 158.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ADENYYKAQTHGK | pY | 535.5618 | 1603.6636 | 3 | 1603.6668 | -0.0032 | 24.94 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 72.0 |  |  |  | A | 1,604.7 | 802.8 | 1,587.6 | 1,586.7 | 13 |
| 2 | 187.1 |  |  | 169.1 | D | 1,533.6 | 767.3 | 1,516.6 | 1,515.6 | 12 |
| 3 | 316.1 |  |  | 298.1 | E | 1,418.6 | 709.8 | 1,401.6 | 1,400.6 | 11 |
| 4 | 430.2 |  | 413.1 | 412.1 | N | 1,289.6 | 645.3 | 1,272.5 | 1,271.6 | 10 |
| 5 | 593.2 |  | 576.2 | 575.2 | $Y$ | 1,175.5 | 588.3 | 1,158.5 | 1,157.5 | 9 |
| 6 | 836.2 | 418.6 | 819.2 | 818.2 | Y+80 | 1,012.5 | 506.7 | 995.4 | 994.5 | 8 |
| 7 | 964.3 | 482.7 | 947.3 | 946.3 | K | 769.4 | 385.2 | 752.4 | 751.4 | 7 |
| 8 | 1,035.4 | 518.2 | 1,018.4 | 1,017.4 | A | 641.3 | 321.2 | 624.3 | 623.3 | 6 |
| 9 | 1,163.4 | 582.2 | 1,146.4 | 1,145.4 | Q | 570.3 | 285.7 | 553.3 | 552.3 | 5 |
| 10 | 1,264.5 | 632.7 | 1,247.5 | 1,246.5 | T | 442.2 | 221.6 | 425.2 | 424.2 | 4 |
| 11 | 1,401.5 | 701.3 | 1,384.5 | 1,383.5 | H | 341.2 | 171.1 | 324.2 |  | 3 |
| 12 | 1,458.6 | 729.8 | 1,441.5 | 1,440.6 | G | 204.1 |  | 187.1 |  | 2 |
| 13 | 1,604.7 | 802.8 | 1,587.6 | 1,586.7 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. $\mathrm{m} / \mathrm{z}$ | Exp. M.W. | Charge | Cal. M.W. | Delta |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| ADENYYKAQTHGK Score |  |  |  |  |  |  |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 72.0 |  |  |  | A | 1,684.6 | 842.8 | 1,667.6 | 1,666.6 | 13 |
| 2 | 187.1 |  |  | 169.1 | D | 1,613.6 | 807.3 | 1,596.6 | 1,595.6 | 12 |
| 3 | 316.1 |  |  | 298.1 | E | 1,498.6 | 749.8 | 1,481.5 | 1,480.6 | 11 |
| 4 | 430.2 |  | 413.1 | 412.1 | N | 1,369.5 | 685.3 | 1,352.5 | 1,351.5 | 10 |
| 5 | 673.2 |  | 656.2 | 655.2 | Y+80 | 1,255.5 | 628.2 | 1,238.5 | 1,237.5 | 9 |
| 6 | 916.2 | 458.6 | 899.2 | 898.2 | Y+80 | 1,012.5 | 506.7 | 995.4 | 994.5 | 8 |
| 7 | 1,044.3 | 522.7 | 1,027.3 | 1,026.3 | K | 769.4 | 385.2 | 752.4 | 751.4 | 7 |
| 8 | 1,115.3 | 558.2 | 1,098.3 | 1,097.3 | A | 641.3 | 321.2 | 624.3 | 623.3 | 6 |
| 9 | 1,243.4 | 622.2 | 1,226.4 | 1,225.4 | Q | 570.3 | 285.7 | 553.3 | 552.3 | 5 |
| 10 | 1,344.5 | 672.7 | 1,327.4 | 1,326.4 | T | 442.2 | 221.6 | 425.2 | 424.2 | 4 |
| 11 | 1,481.5 | 741.3 | 1,464.5 | 1,463.5 | H | 341.2 | 171.1 | 324.2 |  | 3 |
| 12 | 1,538.5 | 769.8 | 1,521.5 | 1,520.5 | G | 204.1 |  | 187.1 |  | 2 |
| 13 | 1,684.6 | 842.8 | 1,667.6 | 1,666.6 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| DNNGŞYALCLLHEGK | pS | 857.3618 | 1712.709 | 2 | 1712.7229 | -0.0139 | 40.03 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 116.0 |  |  | 98.0 | D | 1,713.7 | 857.4 | 1,696.7 | 1,695.7 | 15 |
| 2 | 230.1 |  | 213.1 | 212.1 | N | 1,598.7 | 799.9 | 1,581.7 | 1,580.7 | 14 |
| 3 | 344.1 |  | 327.1 | 326.1 | N | 1,484.7 | 742.8 | 1,467.6 | 1,466.6 | 13 |
| 4 | 401.1 |  | 384.1 | 383.1 | G | 1,370.6 | 685.8 | 1,353.6 | 1,352.6 | 12 |
| 5 | 568.1 |  | 551.1 | 550.1 | S+80 | 1,313.6 | 657.3 | 1,296.6 | 1,295.6 | 11 |
| 6 | 731.2 | 366.1 | 714.2 | 713.2 | Y | 1,146.6 | 573.8 | 1,129.6 | 1,128.6 | 10 |
| 7 | 802.2 | 401.6 | 785.2 | 784.2 | A | 983.5 | 492.3 | 966.5 | 965.5 | 9 |
| 8 | 915.3 | 458.2 | 898.3 | 897.3 | L | 912.5 | 456.8 | 895.5 | 894.5 | 8 |
| 9 | 1,018.3 | 509.7 | 1,001.3 | 1,000.3 | C | 799.4 | 400.2 | 782.4 | 781.4 | 7 |
| 10 | 1,131.4 | 566.2 | 1,114.4 | 1,113.4 | L | 696.4 | 348.7 | 679.4 | 678.4 | 6 |
| 11 | 1,244.5 | 622.8 | 1,227.5 | 1,226.5 | L | 583.3 | 292.2 | 566.3 | 565.3 | 5 |
| 12 | 1,381.6 | 691.3 | 1,364.5 | 1,363.6 | H | 470.2 | 235.6 | 453.2 | 452.2 | 4 |
| 13 | 1,510.6 | 755.8 | 1,493.6 | 1,492.6 | E | 333.2 |  | 316.2 | 315.2 | 3 |
| 14 | 1,567.6 | 784.3 | 1,550.6 | 1,549.6 | G | 204.1 |  | 187.1 |  | 2 |
| 15 | 1,713.7 | 857.4 | 1,696.7 | 1,695.7 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| TGPFEDLKENLIREYVK | pY | 711.0207 | 2130.0403 | 3 | 2130.0398 | 0.0005 | 34.17 |



| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 102.1 |  |  | 84.0 | T | 2,131.0 | 1,066.0 | 2,114.0 | 2,113.0 | 17 |
| 2 | 159.1 |  |  | 141.1 | G | 2,030.0 | 1,015.5 | 2,013.0 | 2,012.0 | 16 |
| 3 | 256.1 |  |  | 238.1 | P | 1,973.0 | 987.0 | 1,956.0 | 1,955.0 | 15 |
| 4 | 403.2 |  |  | 385.2 | F | 1,875.9 | 938.5 | 1,858.9 | 1,857.9 | 14 |
| 5 | 532.2 |  |  | 514.2 | E | 1,728.9 | 864.9 | 1,711.8 | 1,710.8 | 13 |
| 6 | 647.3 | 324.1 |  | 629.3 | D | 1,599.8 | 800.4 | 1,582.8 | 1,581.8 | 12 |
| 7 | 760.4 | 380.7 |  | 742.3 | L | 1,484.8 | 742.9 | 1,467.8 | 1,466.8 | 11 |
| 8 | 888.4 | 444.7 | 871.4 | 870.4 | K | 1,371.7 | 686.4 | 1,354.7 | 1,353.7 | 10 |
| 9 | 1,017.5 | 509.2 | 1,000.5 | 999.5 | E | 1,243.6 | 622.3 | 1,226.6 | 1,225.6 | 9 |
| 10 | 1,131.5 | 566.3 | 1,114.5 | 1,113.5 | N | 1,114.6 | 557.8 | 1,097.5 | 1,096.6 | 8 |
| 11 | 1,244.6 | 622.8 | 1,227.6 | 1,226.6 | L | 1,000.5 | 500.8 | 983.5 | 982.5 | 7 |
| 12 | 1,357.7 | 679.4 | 1,340.7 | 1,339.7 | I | 887.4 | 444.2 | 870.4 | 869.4 | 6 |
| 13 | 1,513.8 | 757.4 | 1,496.8 | 1,495.8 | R | 774.4 | 387.7 | 757.3 | 756.3 | 5 |
| 14 | 1,642.8 | 821.9 | 1,625.8 | 1,624.8 | E | 618.3 |  | 601.2 | 600.2 | 4 |
| 15 | 1,885.9 | 943.4 | 1,868.8 | 1,867.9 | Y+80 | 489.2 |  | 472.2 |  | 3 |
| 16 | 1,984.9 | 993.0 | 1,967.9 | 1,966.9 | Y | 246.2 |  | 229.2 |  | 2 |
| 17 | 2,131.0 | 1,066.0 | 2,114.0 | 2,113.0 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| AssGMADSANHLPFFFGNITR | pS | 774.0195 | 2319.0367 | 3 | 2319.0144 | 0.0223 | 11.65 |



| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 72.0 |  |  |  | A | 2,320.0 | 1,160.5 | 2,303.0 | 2,302.0 | 21 |
| 2 | 159.1 |  |  | 141.1 | S | 2,249.0 | 1,125.0 | 2,232.0 | 2,231.0 | 20 |
| 3 | 326.1 |  |  | 308.1 | S+80 | 2,162.0 | 1,081.5 | 2,144.9 | 2,143.9 | 19 |
| 4 | 383.1 |  |  | 365.1 | G | 1,995.0 | 998.0 | 1,977.9 | 1,976.9 | 18 |
| 5 | 514.1 |  |  | 496.1 | M | 1,937.9 | 969.5 | 1,920.9 | 1,919.9 | 17 |
| 6 | 585.2 | 293.1 |  | 567.2 | A | 1,806.9 | 903.9 | 1,789.9 | 1,788.9 | 16 |
| 7 | 700.2 | 350.6 |  | 682.2 | D | 1,735.9 | 868.4 | 1,718.8 | 1,717.8 | 15 |
| 8 | 787.2 | 394.1 |  | 769.2 | S | 1,620.8 | 810.9 | 1,603.8 | 1,602.8 | 14 |
| 9 | 858.3 | 429.6 |  | 840.3 | A | 1,533.8 | 767.4 | 1,516.8 | 1,515.8 | 13 |
| 10 | 972.3 | 486.7 | 955.3 | 954.3 | N | 1,462.8 | 731.9 | 1,445.7 | 1,444.7 | 12 |
| 11 | 1,109.4 | 555.2 | 1,092.3 | 1,091.4 | H | 1,348.7 | 674.9 | 1,331.7 | 1,330.7 | 11 |
| 12 | 1,222.5 | 611.7 | 1,205.4 | 1,204.4 | L | 1,211.7 | 606.3 | 1,194.6 | 1,193.6 | 10 |
| 13 | 1,319.5 | 660.3 | 1,302.5 | 1,301.5 | P | 1,098.6 | 549.8 | 1,081.5 | 1,080.6 | 9 |
| 14 | 1,466.6 | 733.8 | 1,449.6 | 1,448.6 | F | 1,001.5 | 501.3 | 984.5 | 983.5 | 8 |
| 15 | 1,613.6 | 807.3 | 1,596.6 | 1,595.6 | F | 854.5 | 427.7 | 837.4 | 836.4 | 7 |
| 16 | 1,760.7 | 880.9 | 1,743.7 | 1,742.7 | F | 707.4 | 354.2 | 690.4 | 689.4 | 6 |
| 17 | 1,817.7 | 909.4 | 1,800.7 | 1,799.7 | G | 560.3 |  | 543.3 | 542.3 | 5 |
| 18 | 1,931.8 | 966.4 | 1,914.8 | 1,913.8 | N | 503.3 |  | 486.3 | 485.3 | 4 |
| 19 | 2,044.9 | 1,022.9 | 2,027.8 | 2,026.9 | I | 389.3 |  | 372.2 | 371.2 | 3 |
| 20 | 2,145.9 | 1,073.5 | 2,128.9 | 2,127.9 | T | 276.2 |  | 259.1 | 258.2 | 2 |
| 21 | 2,320.0 | 1,160.5 | 2,303.0 | 2,302.0 | R | 175.1 |  | 158.1 |  |  |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ASSGMADSANHLPFFFGNITR | Mox; pS | 584.7565 | 2334.9969 | 4 | 2335.0093 | -0.0124 | 33.5 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AH | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 72.0 |  |  |  | A | 2,336.0 | 1,168.5 | 2,319.0 | 2,318.0 | 21 |
| 2 | 159.1 |  |  | 141.1 | S | 2,265.0 | 1,133.0 | 2,248.0 | 2,247.0 | 20 |
| 3 | 246.1 |  |  | 228.1 | S | 2,177.9 | 1,089.5 | 2,160.9 | 2,159.9 | 19 |
| 4 | 303.1 |  |  | 285.1 | G | 2,090.9 | 1,046.0 | 2,073.9 | 2,072.9 | 18 |
| 5 | 450.2 |  |  | 432.2 | M+16 | 2,033.9 | 1,017.5 | 2,016.9 | 2,015.9 | 17 |
| 6 | 521.2 | 261.1 |  | 503.2 | A | 1,886.9 | 943.9 | 1,869.8 | 1,868.8 | 16 |
| 7 | 636.2 | 318.6 |  | 618.2 | D | 1,815.8 | 908.4 | 1,798.8 | 1,797.8 | 15 |
| 8 | 803.2 | 402.1 |  | 785.2 | S+80 | 1,700.8 | 850.9 | 1,683.8 | 1,682.8 | 14 |
| 9 | 874.3 | 437.6 |  | 856.3 | A | 1,533.8 | 767.4 | 1,516.8 | 1,515.8 | 13 |
| 10 | 988.3 | 494.7 | 971.3 | 970.3 | N | 1,462.8 | 731.9 | 1,445.7 | 1,444.7 | 12 |
| 11 | 1,125.4 | 563.2 | 1,108.3 | 1,107.4 | H | 1,348.7 | 674.9 | 1,331.7 | 1,330.7 | 11 |
| 12 | 1,238.5 | 619.7 | 1,221.4 | 1,220.4 | L | 1,211.7 | 606.3 | 1,194.6 | 1,193.6 | 10 |
| 13 | 1,335.5 | 668.3 | 1,318.5 | 1,317.5 | P | 1,098.6 | 549.8 | 1,081.5 | 1,080.6 | 9 |
| 14 | 1,482.6 | 741.8 | 1,465.5 | 1,464.6 | F | 1,001.5 | 501.3 | 984.5 | 983.5 | 8 |
| 15 | 1,629.6 | 815.3 | 1,612.6 | 1,611.6 | F | 854.5 | 427.7 | 837.4 | 836.4 | 7 |
| 16 | 1,776.7 | 888.9 | 1,759.7 | 1,758.7 | F | 707.4 | 354.2 | 690.4 | 689.4 | 6 |
| 17 | 1,833.7 | 917.4 | 1,816.7 | 1,815.7 | G | 560.3 |  | 543.3 | 542.3 | 5 |
| 18 | 1,947.8 | 974.4 | 1,930.7 | 1,929.8 | N | 503.3 |  | 486.3 | 485.3 | 4 |
| 19 | 2,060.9 | 1,030.9 | 2,043.8 | 2,042.8 | I | 389.3 |  | 372.2 | 371.2 | 3 |
| 20 | 2,161.9 | 1,081.5 | 2,144.9 | 2,143.9 | T | 276.2 |  | 259.1 | 258.2 | 2 |
| 21 | 2,336.0 | 1,168.5 | 2,319.0 | 2,318.0 | R | 175.1 |  | 158.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| AssGMADSANHLPFFFGNITR | Mox; pS | 779.3511 | 2335.0315 | 3 | 2335.0093 | 0.0222 | 32.38 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AH | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 72.0 |  |  |  | A | 2,336.0 | 1,168.5 | 2,319.0 | 2,318.0 | 21 |
| 2 | 159.1 |  |  | 141.1 | S | 2,265.0 | 1,133.0 | 2,248.0 | 2,247.0 | 20 |
| 3 | 326.1 |  |  | 308.1 | S+80 | 2,177.9 | 1,089.5 | 2,160.9 | 2,159.9 | 19 |
| 4 | 383.1 |  |  | 365.1 | G | 2,010.9 | 1,006.0 | 1,993.9 | 1,992.9 | 18 |
| 5 | 530.1 |  |  | 512.1 | M+16 | 1,953.9 | 977.5 | 1,936.9 | 1,935.9 | 17 |
| 6 | 601.2 | 301.1 |  | 583.2 | A | 1,806.9 | 903.9 | 1,789.9 | 1,788.9 | 16 |
| 7 | 716.2 | 358.6 |  | 698.2 | D | 1,735.9 | 868.4 | 1,718.8 | 1,717.8 | 15 |
| 8 | 803.2 | 402.1 |  | 785.2 | S | 1,620.8 | 810.9 | 1,603.8 | 1,602.8 | 14 |
| 9 | 874.3 | 437.6 |  | 856.3 | A | 1,533.8 | 767.4 | 1,516.8 | 1,515.8 | 13 |
| 10 | 988.3 | 494.7 | 971.3 | 970.3 | N | 1,462.8 | 731.9 | 1,445.7 | 1,444.7 | 12 |
| 11 | 1,125.4 | 563.2 | 1,108.3 | 1,107.4 | H | 1,348.7 | 674.9 | 1,331.7 | 1,330.7 | 11 |
| 12 | 1,238.5 | 619.7 | 1,221.4 | 1,220.4 | L | 1,211.7 | 606.3 | 1,194.6 | 1,193.6 | 10 |
| 13 | 1,335.5 | 668.3 | 1,318.5 | 1,317.5 | P | 1,098.6 | 549.8 | 1,081.5 | 1,080.6 | 9 |
| 14 | 1,482.6 | 741.8 | 1,465.5 | 1,464.6 | F | 1,001.5 | 501.3 | 984.5 | 983.5 | 8 |
| 15 | 1,629.6 | 815.3 | 1,612.6 | 1,611.6 | F | 854.5 | 427.7 | 837.4 | 836.4 | 7 |
| 16 | 1,776.7 | 888.9 | 1,759.7 | 1,758.7 | F | 707.4 | 354.2 | 690.4 | 689.4 | 6 |
| 17 | 1,833.7 | 917.4 | 1,816.7 | 1,815.7 | G | 560.3 |  | 543.3 | 542.3 | 5 |
| 18 | 1,947.8 | 974.4 | 1,930.7 | 1,929.8 | N | 503.3 |  | 486.3 | 485.3 | 4 |
| 19 | 2,060.9 | 1,030.9 | 2,043.8 | 2,042.8 | I | 389.3 |  | 372.2 | 371.2 | 3 |
| 20 | 2,161.9 | 1,081.5 | 2,144.9 | 2,143.9 | T | 276.2 |  | 259.1 | 258.2 | 2 |
| 21 | 2,336.0 | 1,168.5 | 2,319.0 | 2,318.0 | R | 175.1 |  | 158.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| QESTVSFNPYEPELAPWAADK | pY | 1230.042 | 2458.0694 | 2 | 2458.073 | -0.0035 | 48.39 |

y13


| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 129.1 |  | 112.0 |  | Q | 2,459.1 | 1,230.0 | 2,442.1 | 2,441.1 | 21 |
| 2 | 258.1 |  | 241.1 | 240.1 | E | 2,331.0 | 1,166.0 | 2,314.0 | 2,313.0 | 20 |
| 3 | 345.1 |  | 328.1 | 327.1 | S | 2,202.0 | 1,101.5 | 2,185.0 | 2,184.0 | 19 |
| 4 | 446.2 |  | 429.2 | 428.2 | T | 2,114.9 | 1,058.0 | 2,097.9 | 2,096.9 | 18 |
| 5 | 545.3 |  | 528.2 | 527.2 | V | 2,013.9 | 1,007.5 | 1,996.9 | 1,995.9 | 17 |
| 6 | 632.3 | 316.6 | 615.3 | 614.3 | S | 1,914.8 | 957.9 | 1,897.8 | 1,896.8 | 16 |
| 7 | 779.4 | 390.2 | 762.3 | 761.3 | F | 1,827.8 | 914.4 | 1,810.8 | 1,809.8 | 15 |
| 8 | 893.4 | 447.2 | 876.4 | 875.4 | N | 1,680.7 | 840.9 | 1,663.7 | 1,662.7 | 14 |
| 9 | 990.5 | 495.7 | 973.4 | 972.4 | P | 1,566.7 | 783.8 | 1,549.7 | 1,548.7 | 13 |
| 10 | 1,233.5 | 617.2 | 1,216.5 | 1,215.5 | Y+80 | 1,469.6 | 735.3 | 1,452.6 | 1,451.6 | 12 |
| 11 | 1,362.5 | 681.8 | 1,345.5 | 1,344.5 | E | 1,226.6 | 613.8 | 1,209.6 | 1,208.6 | 11 |
| 12 | 1,459.6 | 730.3 | 1,442.6 | 1,441.6 | P | 1,097.6 | 549.3 | 1,080.5 | 1,079.6 | 10 |
| 13 | 1,588.6 | 794.8 | 1,571.6 | 1,570.6 | E | 1,000.5 | 500.8 | 983.5 | 982.5 | 9 |
| 14 | 1,701.7 | 851.4 | 1,684.7 | 1,683.7 | L | 871.5 | 436.2 | 854.4 | 853.5 | 8 |
| 15 | 1,772.7 | 886.9 | 1,755.7 | 1,754.7 | A | 758.4 | 379.7 | 741.4 | 740.4 | 7 |
| 16 | 1,869.8 | 935.4 | 1,852.8 | 1,851.8 | P | 687.3 | 344.2 | 670.3 | 669.3 | 6 |
| 17 | 2,055.9 | 1,028.4 | 2,038.8 | 2,037.9 | W | 590.3 |  | 573.3 | 572.3 | 5 |
| 18 | 2,126.9 | 1,064.0 | 2,109.9 | 2,108.9 | A | 404.2 |  | 387.2 | 386.2 | 4 |
| 19 | 2,197.9 | 1,099.5 | 2,180.9 | 2,179.9 | A | 333.2 |  | 316.2 | 315.2 | 3 |
| 20 | 2,313.0 | 1,157.0 | 2,295.9 | 2,295.0 | D | 262.1 |  | 245.1 | 244.1 | 2 |
| 21 | 2,459.1 | 1,230.0 | 2,442.1 | 2,441.1 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| EALPMDTEVYESPYADPEEIRPK | Mox; pY | 1388.107 | 2774.1994 | 2 | 2774.2034 | -0.0039 | 49.52 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 130.0 |  |  | 112.0 | E | 2,775.2 | 1,388.1 | 2,758.2 | 2,757.2 | 23 |
| 2 | 201.1 |  |  | 183.1 | A | 2,646.2 | 1,323.6 | 2,629.1 | 2,628.2 | 22 |
| 3 | 314.2 |  |  | 296.2 | L | 2,575.1 | 1,288.1 | 2,558.1 | 2,557.1 | 21 |
| 4 | 411.2 |  |  | 393.2 | P | 2,462.0 | 1,231.5 | 2,445.0 | 2,444.0 | 20 |
| 5 | 558.3 |  |  | 540.2 | M+16 | 2,365.0 | 1,183.0 | 2,348.0 | 2,347.0 | 19 |
| 6 | 673.3 | 337.1 |  | 655.3 | D | 2,218.0 | 1,109.5 | 2,200.9 | 2,199.9 | 18 |
| 7 | 774.3 | 387.7 |  | 756.3 | T | 2,102.9 | 1,052.0 | 2,085.9 | 2,084.9 | 17 |
| 8 | 903.4 | 452.2 |  | 885.4 | E | 2,001.9 | 1,001.4 | 1,984.9 | 1,983.9 | 16 |
| 9 | 1,002.4 | 501.7 |  | 984.4 | V | 1,872.8 | 936.9 | 1,855.8 | 1,854.8 | 15 |
| 10 | 1,165.5 | 583.3 |  | 1,147.5 | $Y$ | 1,773.8 | 887.4 | 1,756.7 | 1,755.8 | 14 |
| 11 | 1,294.6 | 647.8 |  | 1,276.5 | E | 1,610.7 | 805.9 | 1,593.7 | 1,592.7 | 13 |
| 12 | 1,381.6 | 691.3 |  | 1,363.6 | S | 1,481.7 | 741.3 | 1,464.6 | 1,463.7 | 12 |
| 13 | 1,478.6 | 739.8 |  | 1,460.6 | P | 1,394.6 | 697.8 | 1,377.6 | 1,376.6 | 11 |
| 14 | 1,721.7 | 861.3 |  | 1,703.7 | Y+80 | 1,297.6 | 649.3 | 1,280.6 | 1,279.6 | 10 |
| 15 | 1,792.7 | 896.9 |  | 1,774.7 | A | 1,054.6 | 527.8 | 1,037.5 | 1,036.5 | 9 |
| 16 | 1,907.7 | 954.4 |  | 1,889.7 | D | 983.5 | 492.3 | 966.5 | 965.5 | 8 |
| 17 | 2,004.8 | 1,002.9 |  | 1,986.8 | P | 868.5 | 434.7 | 851.5 | 850.5 | 7 |
| 18 | 2,133.8 | 1,067.4 |  | 2,115.8 | E | 771.4 | 386.2 | 754.4 | 753.4 | 6 |
| 19 | 2,262.9 | 1,131.9 |  | 2,244.9 | E | 642.4 | 321.7 | 625.4 | 624.4 | 5 |
| 20 | 2,376.0 | 1,188.5 |  | 2,357.9 | I | 513.4 | 257.2 | 496.3 |  | 4 |
| 21 | 2,532.1 | 1,266.5 | 2,515.0 | 2,514.0 | R | 400.3 | 200.6 | 383.2 |  | 3 |
| 22 | 2,629.1 | 1,315.1 | 2,612.1 | 2,611.1 | P | 244.2 |  | 227.1 |  | 2 |
| 23 | 2,775.2 | 1,388.1 | 2,758.2 | 2,757.2 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| EALPMDTEVYESPYADPEEIRPK | Mox; pY | 925.7414 | 2774.2024 | 3 | 2774.2034 | -0.001 | 36.85 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 130.0 |  |  | 112.0 | E | 2,775.2 | 1,388.1 | 2,758.2 | 2,757.2 | 23 |
| 2 | 201.1 |  |  | 183.1 | A | 2,646.2 | 1,323.6 | 2,629.1 | 2,628.2 | 22 |
| 3 | 314.2 |  |  | 296.2 | L | 2,575.1 | 1,288.1 | 2,558.1 | 2,557.1 | 21 |
| 4 | 411.2 |  |  | 393.2 | P | 2,462.0 | 1,231.5 | 2,445.0 | 2,444.0 | 20 |
| 5 | 558.3 |  |  | 540.2 | M+16 | 2,365.0 | 1,183.0 | 2,348.0 | 2,347.0 | 19 |
| 6 | 673.3 | 337.1 |  | 655.3 | D | 2,218.0 | 1,109.5 | 2,200.9 | 2,199.9 | 18 |
| 7 | 774.3 | 387.7 |  | 756.3 | T | 2,102.9 | 1,052.0 | 2,085.9 | 2,084.9 | 17 |
| 8 | 903.4 | 452.2 |  | 885.4 | E | 2,001.9 | 1,001.4 | 1,984.9 | 1,983.9 | 16 |
| 9 | 1,002.4 | 501.7 |  | 984.4 | Y | 1,872.8 | 936.9 | 1,855.8 | 1,854.8 | 15 |
| 10 | 1,245.5 | 623.2 |  | 1,227.5 | Y+80 | 1,773.8 | 887.4 | 1,756.7 | 1,755.8 | 14 |
| 11 | 1,374.5 | 687.8 |  | 1,356.5 | E | 1,530.7 | 765.9 | 1,513.7 | 1,512.7 | 13 |
| 12 | 1,461.5 | 731.3 |  | 1,443.5 | S | 1,401.7 | 701.4 | 1,384.7 | 1,383.7 | 12 |
| 13 | 1,558.6 | 779.8 |  | 1,540.6 | P | 1,314.7 | 657.8 | 1,297.6 | 1,296.7 | 11 |
| 14 | 1,721.7 | 861.3 |  | 1,703.7 | $Y$ | 1,217.6 | 609.3 | 1,200.6 | 1,199.6 | 10 |
| 15 | 1,792.7 | 896.9 |  | 1,774.7 | A | 1,054.6 | 527.8 | 1,037.5 | 1,036.5 | 9 |
| 16 | 1,907.7 | 954.4 |  | 1,889.7 | D | 983.5 | 492.3 | 966.5 | 965.5 | 8 |
| 17 | 2,004.8 | 1,002.9 |  | 1,986.8 | P | 868.5 | 434.7 | 851.5 | 850.5 | 7 |
| 18 | 2,133.8 | 1,067.4 |  | 2,115.8 | E | 771.4 | 386.2 | 754.4 | 753.4 | 6 |
| 19 | 2,262.9 | 1,131.9 |  | 2,244.9 | E | 642.4 | 321.7 | 625.4 | 624.4 | 5 |
| 20 | 2,376.0 | 1,188.5 |  | 2,357.9 | I | 513.4 | 257.2 | 496.3 |  | 4 |
| 21 | 2,532.1 | 1,266.5 | 2,515.0 | 2,514.0 | R | 400.3 | 200.6 | 383.2 |  | 3 |
| 22 | 2,629.1 | 1,315.1 | 2,612.1 | 2,611.1 | P | 244.2 |  | 227.1 |  | 2 |
| 23 | 2,775.2 | 1,388.1 | 2,758.2 | 2,757.2 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. $\mathrm{m} / \mathrm{z}$ | Exp. M.W. | Charge | Cal. M.W. | Delta |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| EALPMDTEVYESPYYADPEEIRPK | Mox; pS | 925.7446 | 2774.212 | 3 | 2774.2034 | 0.0086 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 130.0 |  |  | 112.0 | E | 2,775.2 | 1,388.1 | 2,758.2 | 2,757.2 | 23 |
| 2 | 201.1 |  |  | 183.1 | A | 2,646.2 | 1,323.6 | 2,629.1 | 2,628.2 | 22 |
| 3 | 314.2 |  |  | 296.2 | L | 2,575.1 | 1,288.1 | 2,558.1 | 2,557.1 | 21 |
| 4 | 411.2 |  |  | 393.2 | P | 2,462.0 | 1,231.5 | 2,445.0 | 2,444.0 | 20 |
| 5 | 558.3 |  |  | 540.2 | M+16 | 2,365.0 | 1,183.0 | 2,348.0 | 2,347.0 | 19 |
| 6 | 673.3 | 337.1 |  | 655.3 | D | 2,218.0 | 1,109.5 | 2,200.9 | 2,199.9 | 18 |
| 7 | 774.3 | 387.7 |  | 756.3 | T | 2,102.9 | 1,052.0 | 2,085.9 | 2,084.9 | 17 |
| 8 | 903.4 | 452.2 |  | 885.4 | E | 2,001.9 | 1,001.4 | 1,984.9 | 1,983.9 | 16 |
| 9 | 1,002.4 | 501.7 |  | 984.4 | Y | 1,872.8 | 936.9 | 1,855.8 | 1,854.8 | 15 |
| 10 | 1,165.5 | 583.3 |  | 1,147.5 | $Y$ | 1,773.8 | 887.4 | 1,756.7 | 1,755.8 | 14 |
| 11 | 1,294.6 | 647.8 |  | 1,276.5 | E | 1,610.7 | 805.9 | 1,593.7 | 1,592.7 | 13 |
| 12 | 1,461.5 | 731.3 |  | 1,443.5 | S+80 | 1,481.7 | 741.3 | 1,464.6 | 1,463.7 | 12 |
| 13 | 1,558.6 | 779.8 |  | 1,540.6 | P | 1,314.7 | 657.8 | 1,297.6 | 1,296.7 | 11 |
| 14 | 1,721.7 | 861.3 |  | 1,703.7 | $Y$ | 1,217.6 | 609.3 | 1,200.6 | 1,199.6 | 10 |
| 15 | 1,792.7 | 896.9 |  | 1,774.7 | A | 1,054.6 | 527.8 | 1,037.5 | 1,036.5 | 9 |
| 16 | 1,907.7 | 954.4 |  | 1,889.7 | D | 983.5 | 492.3 | 966.5 | 965.5 | 8 |
| 17 | 2,004.8 | 1,002.9 |  | 1,986.8 | P | 868.5 | 434.7 | 851.5 | 850.5 | 7 |
| 18 | 2,133.8 | 1,067.4 |  | 2,115.8 | E | 771.4 | 386.2 | 754.4 | 753.4 | 6 |
| 19 | 2,262.9 | 1,131.9 |  | 2,244.9 | E | 642.4 | 321.7 | 625.4 | 624.4 | 5 |
| 20 | 2,376.0 | 1,188.5 |  | 2,357.9 | I | 513.4 | 257.2 | 496.3 |  | 4 |
| 21 | 2,532.1 | 1,266.5 | 2,515.0 | 2,514.0 | R | 400.3 | 200.6 | 383.2 |  | 3 |
| 22 | 2,629.1 | 1,315.1 | 2,612.1 | 2,611.1 | P | 244.2 |  | 227.1 |  | 2 |
| 23 | 2,775.2 | 1,388.1 | 2,758.2 | 2,757.2 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| MIGICEAESWMLVMEMAELGPLNK | 2 Mox; pS | 936.4166 | 2806.228 | 3 | 2806.216 | 0.0119 | 20.16 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 132.0 |  |  |  | M | 2,807.2 | 1,404.1 | 2,790.2 | 2,789.2 | 24 |
| 2 | 245.1 |  |  |  | I | 2,676.2 | 1,338.6 | 2,659.2 | 2,658.2 | 23 |
| 3 | 302.2 |  |  |  | G | 2,563.1 | 1,282.1 | 2,546.1 | 2,545.1 | 22 |
| 4 | 415.2 |  |  |  | I | 2,506.1 | 1,253.5 | 2,489.1 | 2,488.1 | 21 |
| 5 | 518.2 |  |  |  | C | 2,393.0 | 1,197.0 | 2,376.0 | 2,375.0 | 20 |
| 6 | 647.3 | 324.1 |  | 629.3 | E | 2,290.0 | 1,145.5 | 2,273.0 | 2,272.0 | 19 |
| 7 | 718.3 | 359.7 |  | 700.3 | A | 2,160.9 | 1,081.0 | 2,143.9 | 2,142.9 | 18 |
| 8 | 847.4 | 424.2 |  | 829.4 | E | 2,089.9 | 1,045.5 | 2,072.9 | 2,071.9 | 17 |
| 9 | 1,014.4 | 507.7 |  | 996.4 | S+80 | 1,960.9 | 980.9 | 1,943.8 | 1,942.9 | 16 |
| 10 | 1,200.4 | 600.7 |  | 1,182.4 | W | 1,793.9 | 897.4 | 1,776.8 | 1,775.9 | 15 |
| 11 | 1,331.5 | 666.2 |  | 1,313.5 | M | 1,607.8 | 804.4 | 1,590.8 | 1,589.8 | 14 |
| 12 | 1,444.6 | 722.8 |  | 1,426.6 | L | 1,476.7 | 738.9 | 1,459.7 | 1,458.7 | 13 |
| 13 | 1,543.6 | 772.3 |  | 1,525.6 | Y | 1,363.7 | 682.3 | 1,346.6 | 1,345.6 | 12 |
| 14 | 1,690.7 | 845.8 |  | 1,672.7 | M+16 | 1,264.6 | 632.8 | 1,247.6 | 1,246.6 | 11 |
| 15 | 1,819.7 | 910.4 |  | 1,801.7 | E | 1,117.6 | 559.3 | 1,100.5 | 1,099.5 | 10 |
| 16 | 1,966.8 | 983.9 |  | 1,948.7 | M+16 | 988.5 | 494.8 | 971.5 | 970.5 | 9 |
| 17 | 2,037.8 | 1,019.4 |  | 2,019.8 | A | 841.5 | 421.2 | 824.5 | 823.5 | 8 |
| 18 | 2,166.8 | 1,083.9 |  | 2,148.8 | E | 770.4 | 385.7 | 753.4 | 752.4 | 7 |
| 19 | 2,279.9 | 1,140.5 |  | 2,261.9 | L | 641.4 | 321.2 | 624.4 |  | 6 |
| 20 | 2,336.9 | 1,169.0 |  | 2,318.9 | G | 528.3 |  | 511.3 |  | 5 |
| 21 | 2,434.0 | 1,217.5 |  | 2,416.0 | P | 471.3 |  | 454.3 |  | 4 |
| 22 | 2,547.1 | 1,274.0 |  | 2,529.1 | L | 374.2 |  | 357.2 |  | 3 |
| 23 | 2,661.1 | 1,331.1 | 2,644.1 | 2,643.1 | N | 261.2 |  | 244.1 |  | 2 |
| 24 | 2,807.2 | 1,404.1 | 2,790.2 | 2,789.2 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| EALPMDTEVYESPYADPEEIRPK | 2 pY | 947.0668 | 2838.1786 | 3 | 2838.1748 | 0.0038 | 61.19 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 130.0 |  |  | 112.0 | E | 2,839.2 | 1,420.1 | 2,822.2 | 2,821.2 | 23 |
| 2 | 201.1 |  |  | 183.1 | A | 2,710.1 | 1,355.6 | 2,693.1 | 2,692.1 | 22 |
| 3 | 314.2 |  |  | 296.2 | L | 2,639.1 | 1,320.1 | 2,622.1 | 2,621.1 | 21 |
| 4 | 411.2 |  |  | 393.2 | P | 2,526.0 | 1,263.5 | 2,509.0 | 2,508.0 | 20 |
| 5 | 542.3 |  |  | 524.3 | M | 2,429.0 | 1,215.0 | 2,411.9 | 2,411.0 | 19 |
| 6 | 657.3 | 329.1 |  | 639.3 | D | 2,297.9 | 1,149.5 | 2,280.9 | 2,279.9 | 18 |
| 7 | 758.3 | 379.7 |  | 740.3 | T | 2,182.9 | 1,092.0 | 2,165.9 | 2,164.9 | 17 |
| 8 | 887.4 | 444.2 |  | 869.4 | E | 2,081.9 | 1,041.4 | 2,064.8 | 2,063.8 | 16 |
| 9 | 986.5 | 493.7 |  | 968.4 | Y | 1,952.8 | 976.9 | 1,935.8 | 1,934.8 | 15 |
| 10 | 1,229.5 | 615.2 |  | 1,211.5 | Y+80 | 1,853.7 | 927.4 | 1,836.7 | 1,835.7 | 14 |
| 11 | 1,358.5 | 679.8 |  | 1,340.5 | E | 1,610.7 | 805.9 | 1,593.7 | 1,592.7 | 13 |
| 12 | 1,445.6 | 723.3 |  | 1,427.5 | S | 1,481.7 | 741.3 | 1,464.6 | 1,463.7 | 12 |
| 13 | 1,542.6 | 771.8 |  | 1,524.6 | P | 1,394.6 | 697.8 | 1,377.6 | 1,376.6 | 11 |
| 14 | 1,785.6 | 893.3 |  | 1,767.6 | Y+80 | 1,297.6 | 649.3 | 1,280.6 | 1,279.6 | 10 |
| 15 | 1,856.7 | 928.8 |  | 1,838.7 | A | 1,054.6 | 527.8 | 1,037.5 | 1,036.5 | 9 |
| 16 | 1,971.7 | 986.4 |  | 1,953.7 | D | 983.5 | 492.3 | 966.5 | 965.5 | 8 |
| 17 | 2,068.8 | 1,034.9 |  | 2,050.7 | P | 868.5 | 434.7 | 851.5 | 850.5 | 7 |
| 18 | 2,197.8 | 1,099.4 |  | 2,179.8 | E | 771.4 | 386.2 | 754.4 | 753.4 | 6 |
| 19 | 2,326.8 | 1,163.9 |  | 2,308.8 | E | 642.4 | 321.7 | 625.4 | 624.4 | 5 |
| 20 | 2,439.9 | 1,220.5 |  | 2,421.9 | I | 513.4 | 257.2 | 496.3 |  | 4 |
| 21 | 2,596.0 | 1,298.5 | 2,579.0 | 2,578.0 | R | 400.3 | 200.6 | 383.2 |  | 3 |
| 22 | 2,693.1 | 1,347.0 | 2,676.1 | 2,675.1 | P | 244.2 |  | 227.1 |  | 2 |
| 23 | 2,839.2 | 1,420.1 | 2,822.2 | 2,821.2 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| MIGICEAESWMLVMEMAELGPLNK | 4 Mox; pS | 947.0814 | 2838.2224 | 3 | 2838.2059 | 0.0165 | 26.19 |



| B | $B$ Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 148.0 |  |  |  | M+16 | 2,839.2 | 1,420.1 | 2,822.2 | 2,821.2 | 24 |
| 2 | 261.1 |  |  |  | I | 2,692.2 | 1,346.6 | 2,675.2 | 2,674.2 | 23 |
| 3 | 318.1 |  |  |  | G | 2,579.1 | 1,290.1 | 2,562.1 | 2,561.1 | 22 |
| 4 | 431.2 |  |  |  | I | 2,522.1 | 1,261.5 | 2,505.0 | 2,504.1 | 21 |
| 5 | 534.2 |  |  |  | C | 2,409.0 | 1,205.0 | 2,392.0 | 2,391.0 | 20 |
| 6 | 663.3 | 332.1 |  | 645.3 | E | 2,306.0 | 1,153.5 | 2,289.0 | 2,288.0 | 19 |
| 7 | 734.3 | 367.7 |  | 716.3 | A | 2,176.9 | 1,089.0 | 2,159.9 | 2,158.9 | 18 |
| 8 | 863.4 | 432.2 |  | 845.4 | E | 2,105.9 | 1,053.5 | 2,088.9 | 2,087.9 | 17 |
| 9 | 1,030.4 | 515.7 |  | 1,012.4 | S+80 | 1,976.9 | 988.9 | 1,959.8 | 1,958.8 | 16 |
| 10 | 1,216.4 | 608.7 |  | 1,198.4 | W | 1,809.9 | 905.4 | 1,792.8 | 1,791.8 | 15 |
| 11 | 1,363.5 | 682.2 |  | 1,345.5 | M+16 | 1,623.8 | 812.4 | 1,606.8 | 1,605.8 | 14 |
| 12 | 1,476.6 | 738.8 |  | 1,458.6 | L | 1,476.7 | 738.9 | 1,459.7 | 1,458.7 | 13 |
| 13 | 1,575.6 | 788.3 |  | 1,557.6 | V | 1,363.7 | 682.3 | 1,346.6 | 1,345.6 | 12 |
| 14 | 1,722.7 | 861.8 |  | 1,704.7 | M+16 | 1,264.6 | 632.8 | 1,247.6 | 1,246.6 | 11 |
| 15 | 1,851.7 | 926.4 |  | 1,833.7 | E | 1,117.6 | 559.3 | 1,100.5 | 1,099.5 | 10 |
| 16 | 1,998.7 | 999.9 |  | 1,980.7 | M+16 | 988.5 | 494.8 | 971.5 | 970.5 | 9 |
| 17 | 2,069.8 | 1,035.4 |  | 2,051.8 | A | 841.5 | 421.2 | 824.5 | 823.5 | 8 |
| 18 | 2,198.8 | 1,099.9 |  | 2,180.8 | E | 770.4 | 385.7 | 753.4 | 752.4 | 7 |
| 19 | 2,311.9 | 1,156.5 |  | 2,293.9 | L | 641.4 | 321.2 | 624.4 |  | 6 |
| 20 | 2,368.9 | 1,185.0 |  | 2,350.9 | G | 528.3 |  | 511.3 |  | 5 |
| 21 | 2,466.0 | 1,233.5 |  | 2,448.0 | P | 471.3 |  | 454.3 |  | 4 |
| 22 | 2,579.1 | 1,290.0 |  | 2,561.1 | L | 374.2 |  | 357.2 |  | 3 |
| 23 | 2,693.1 | 1,347.1 | 2,676.1 | 2,675.1 | N | 261.2 |  | 244.1 |  | 2 |
| 24 | 2,839.2 | 1,420.1 | 2,822.2 | 2,821.2 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| EALPMDTEVYESPYADPEEIRPK | Mox; 2 pY | 952.3978 | 2854.1716 | 3 | 2854.1697 | 0.0019 | 59.45 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 130.0 |  |  | 112.0 | E | 2,855.2 | 1,428.1 | 2,838.2 | 2,837.2 | 23 |
| 2 | 201.1 |  |  | 183.1 | A | 2,726.1 | 1,363.6 | 2,709.1 | 2,708.1 | 22 |
| 3 | 314.2 |  |  | 296.2 | L | 2,655.1 | 1,328.1 | 2,638.1 | 2,637.1 | 21 |
| 4 | 411.2 |  |  | 393.2 | P | 2,542.0 | 1,271.5 | 2,525.0 | 2,524.0 | 20 |
| 5 | 558.3 |  |  | 540.2 | M+16 | 2,445.0 | 1,223.0 | 2,427.9 | 2,427.0 | 19 |
| 6 | 673.3 | 337.1 |  | 655.3 | D | 2,297.9 | 1,149.5 | 2,280.9 | 2,279.9 | 18 |
| 7 | 774.3 | 387.7 |  | 756.3 | T | 2,182.9 | 1,092.0 | 2,165.9 | 2,164.9 | 17 |
| 8 | 903.4 | 452.2 |  | 885.4 | E | 2,081.9 | 1,041.4 | 2,064.8 | 2,063.8 | 16 |
| 9 | 1,002.4 | 501.7 |  | 984.4 | Y | 1,952.8 | 976.9 | 1,935.8 | 1,934.8 | 15 |
| 10 | 1,245.5 | 623.2 |  | 1,227.5 | Y+80 | 1,853.7 | 927.4 | 1,836.7 | 1,835.7 | 14 |
| 11 | 1,374.5 | 687.8 |  | 1,356.5 | E | 1,610.7 | 805.9 | 1,593.7 | 1,592.7 | 13 |
| 12 | 1,461.5 | 731.3 |  | 1,443.5 | S | 1,481.7 | 741.3 | 1,464.6 | 1,463.7 | 12 |
| 13 | 1,558.6 | 779.8 |  | 1,540.6 | P | 1,394.6 | 697.8 | 1,377.6 | 1,376.6 | 11 |
| 14 | 1,801.6 | 901.3 |  | 1,783.6 | Y+80 | 1,297.6 | 649.3 | 1,280.6 | 1,279.6 | 10 |
| 15 | 1,872.7 | 936.8 |  | 1,854.7 | A | 1,054.6 | 527.8 | 1,037.5 | 1,036.5 | 9 |
| 16 | 1,987.7 | 994.4 |  | 1,969.7 | D | 983.5 | 492.3 | 966.5 | 965.5 | 8 |
| 17 | 2,084.7 | 1,042.9 |  | 2,066.7 | P | 868.5 | 434.7 | 851.5 | 850.5 | 7 |
| 18 | 2,213.8 | 1,107.4 |  | 2,195.8 | E | 771.4 | 386.2 | 754.4 | 753.4 | 6 |
| 19 | 2,342.8 | 1,171.9 |  | 2,324.8 | E | 642.4 | 321.7 | 625.4 | 624.4 | 5 |
| 20 | 2,455.9 | 1,228.5 |  | 2,437.9 | 1 | 513.4 | 257.2 | 496.3 |  | 4 |
| 21 | 2,612.0 | 1,306.5 | 2,595.0 | 2,594.0 | R | 400.3 | 200.6 | 383.2 |  | 3 |
| 22 | 2,709.1 | 1,355.0 | 2,692.0 | 2,691.1 | P | 244.2 |  | 227.1 |  | 2 |
| 23 | 2,855.2 | 1,428.1 | 2,838.2 | 2,837.2 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| EALPMDTEVYESPYYADPEEIRPK | Mox; pS; pY | 952.3985 | 2854.1737 | 3 | 2854.1697 | 0.004 | 21.26 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 130.0 |  |  | 112.0 | E | 2,855.2 | 1,428.1 | 2,838.2 | 2,837.2 | 23 |
| 2 | 201.1 |  |  | 183.1 | A | 2,726.1 | 1,363.6 | 2,709.1 | 2,708.1 | 22 |
| 3 | 314.2 |  |  | 296.2 | L | 2,655.1 | 1,328.1 | 2,638.1 | 2,637.1 | 21 |
| 4 | 411.2 |  |  | 393.2 | P | 2,542.0 | 1,271.5 | 2,525.0 | 2,524.0 | 20 |
| 5 | 558.3 |  |  | 540.2 | M+16 | 2,445.0 | 1,223.0 | 2,427.9 | 2,427.0 | 19 |
| 6 | 673.3 | 337.1 |  | 655.3 | D | 2,297.9 | 1,149.5 | 2,280.9 | 2,279.9 | 18 |
| 7 | 774.3 | 387.7 |  | 756.3 | T | 2,182.9 | 1,092.0 | 2,165.9 | 2,164.9 | 17 |
| 8 | 903.4 | 452.2 |  | 885.4 | E | 2,081.9 | 1,041.4 | 2,064.8 | 2,063.8 | 16 |
| 9 | 1,002.4 | 501.7 |  | 984.4 | Y | 1,952.8 | 976.9 | 1,935.8 | 1,934.8 | 15 |
| 10 | 1,165.5 | 583.3 |  | 1,147.5 | $Y$ | 1,853.7 | 927.4 | 1,836.7 | 1,835.7 | 14 |
| 11 | 1,294.6 | 647.8 |  | 1,276.5 | E | 1,690.7 | 845.8 | 1,673.6 | 1,672.7 | 13 |
| 12 | 1,461.5 | 731.3 |  | 1,443.5 | S+80 | 1,561.6 | 781.3 | 1,544.6 | 1,543.6 | 12 |
| 13 | 1,558.6 | 779.8 |  | 1,540.6 | P | 1,394.6 | 697.8 | 1,377.6 | 1,376.6 | 11 |
| 14 | 1,801.6 | 901.3 |  | 1,783.6 | Y+80 | 1,297.6 | 649.3 | 1,280.6 | 1,279.6 | 10 |
| 15 | 1,872.7 | 936.8 |  | 1,854.7 | A | 1,054.6 | 527.8 | 1,037.5 | 1,036.5 | 9 |
| 16 | 1,987.7 | 994.4 |  | 1,969.7 | D | 983.5 | 492.3 | 966.5 | 965.5 | 8 |
| 17 | 2,084.7 | 1,042.9 |  | 2,066.7 | P | 868.5 | 434.7 | 851.5 | 850.5 | 7 |
| 18 | 2,213.8 | 1,107.4 |  | 2,195.8 | E | 771.4 | 386.2 | 754.4 | 753.4 | 6 |
| 19 | 2,342.8 | 1,171.9 |  | 2,324.8 | E | 642.4 | 321.7 | 625.4 | 624.4 | 5 |
| 20 | 2,455.9 | 1,228.5 |  | 2,437.9 | I | 513.4 | 257.2 | 496.3 |  | 4 |
| 21 | 2,612.0 | 1,306.5 | 2,595.0 | 2,594.0 | R | 400.3 | 200.6 | 383.2 |  | 3 |
| 22 | 2,709.1 | 1,355.0 | 2,692.0 | 2,691.1 | P | 244.2 |  | 227.1 |  | 2 |
| 23 | 2,855.2 | 1,428.1 | 2,838.2 | 2,837.2 | K | 147.1 |  | 130.1 |  | , |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| QESTVSFNPYEPELAPWAADKGPQR | pY | 966.4431 | 2896.3075 | 3 | 2896.3069 | 0.0006 | 82.45 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 129.1 |  | 112.0 |  | Q | 2,897.3 | 1,449.2 | 2,880.3 | 2,879.3 | 25 |
| 2 | 258.1 |  | 241.1 | 240.1 | E | 2,769.3 | 1,385.1 | 2,752.2 | 2,751.2 | 24 |
| 3 | 345.1 |  | 328.1 | 327.1 | S | 2,640.2 | 1,320.6 | 2,623.2 | 2,622.2 | 23 |
| 4 | 446.2 |  | 429.2 | 428.2 | T | 2,553.2 | 1,277.1 | 2,536.2 | 2,535.2 | 22 |
| 5 | 545.3 |  | 528.2 | 527.2 | Y | 2,452.1 | 1,226.6 | 2,435.1 | 2,434.1 | 21 |
| 6 | 632.3 | 316.6 | 615.3 | 614.3 | S | 2,353.1 | 1,177.0 | 2,336.0 | 2,335.1 | 20 |
| 7 | 779.4 | 390.2 | 762.3 | 761.3 | F | 2,266.0 | 1,133.5 | 2,249.0 | 2,248.0 | 19 |
| 8 | 893.4 | 447.2 | 876.4 | 875.4 | N | 2,119.0 | 1,060.0 | 2,101.9 | 2,101.0 | 18 |
| 9 | 990.5 | 495.7 | 973.4 | 972.4 | P | 2,004.9 | 1,003.0 | 1,987.9 | 1,986.9 | 17 |
| 10 | 1,233.5 | 617.2 | 1,216.5 | 1,215.5 | $Y+80$ | 1,907.9 | 954.4 | 1,890.8 | 1,889.9 | 16 |
| 11 | 1,362.5 | 681.8 | 1,345.5 | 1,344.5 | E | 1,664.8 | 832.9 | 1,647.8 | 1,646.8 | 15 |
| 12 | 1,459.6 | 730.3 | 1,442.6 | 1,441.6 | P | 1,535.8 | 768.4 | 1,518.8 | 1,517.8 | 14 |
| 13 | 1,588.6 | 794.8 | 1,571.6 | 1,570.6 | E | 1,438.7 | 719.9 | 1,421.7 | 1,420.7 | 13 |
| 14 | 1,701.7 | 851.4 | 1,684.7 | 1,683.7 | L | 1,309.7 | 655.4 | 1,292.7 | 1,291.7 | 12 |
| 15 | 1,772.7 | 886.9 | 1,755.7 | 1,754.7 | A | 1,196.6 | 598.8 | 1,179.6 | 1,178.6 | 11 |
| 16 | 1,869.8 | 935.4 | 1,852.8 | 1,851.8 | P | 1,125.6 | 563.3 | 1,108.6 | 1,107.6 | 10 |
| 17 | 2,055.9 | 1,028.4 | 2,038.8 | 2,037.9 | W | 1,028.5 | 514.8 | 1,011.5 | 1,010.5 | 9 |
| 18 | 2,126.9 | 1,064.0 | 2,109.9 | 2,108.9 | A | 842.4 | 421.7 | 825.4 | 824.4 | 8 |
| 19 | 2,197.9 | 1,099.5 | 2,180.9 | 2,179.9 | A | 771.4 | 386.2 | 754.4 | 753.4 | 7 |
| 20 | 2,313.0 | 1,157.0 | 2,295.9 | 2,295.0 | D | 700.4 | 350.7 | 683.3 | 682.4 | 6 |
| 21 | 2,441.1 | 1,221.0 | 2,424.0 | 2,423.1 | K | 585.3 | 293.2 | 568.3 |  | 5 |
| 22 | 2,498.1 | 1,249.5 | 2,481.1 | 2,480.1 | G | 457.3 |  | 440.2 |  | 4 |
| 23 | 2,595.1 | 1,298.1 | 2,578.1 | 2,577.1 | P | 400.2 |  | 383.2 |  | 3 |
| 24 | 2,723.2 | 1,362.1 | 2,706.2 | 2,705.2 | Q | 303.2 |  | 286.2 |  | 2 |
| 25 | 2,897.3 | 1,449.2 | 2,880.3 | 2,879.3 | R | 175.1 |  | 158.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| EMYDLMNLCWTYDVENRPGFAAVELR | 2 Mox; pT | 1083.139 | 3246.3952 | 3 | 3246.3861 | 0.009 | 49.45 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 130.0 |  |  | 112.0 | E | 3,247.4 | 1,624.2 | 3,230.4 | 3,229.4 | 26 |
| 2 | 277.1 |  |  | 259.1 | M+16 | 3,118.4 | 1,559.7 | 3,101.3 | 3,100.3 | 25 |
| 3 | 440.1 |  |  | 422.1 | Y | 2,971.3 | 1,486.2 | 2,954.3 | 2,953.3 | 24 |
| 4 | 555.2 |  |  | 537.2 | D | 2,808.3 | 1,404.6 | 2,791.2 | 2,790.2 | 23 |
| 5 | 668.3 |  |  | 650.2 | L | 2,693.2 | 1,347.1 | 2,676.2 | 2,675.2 | 22 |
| 6 | 815.3 | 408.2 |  | 797.3 | M+16 | 2,580.1 | 1,290.6 | 2,563.1 | 2,562.1 | 21 |
| 7 | 929.3 | 465.2 | 912.3 | 911.3 | N | 2,433.1 | 1,217.1 | 2,416.1 | 2,415.1 | 20 |
| 8 | 1,042.4 | 521.7 | 1,025.4 | 1,024.4 | L | 2,319.1 | 1,160.0 | 2,302.0 | 2,301.1 | 19 |
| 9 | 1,145.4 | 573.2 | 1,128.4 | 1,127.4 | C | 2,206.0 | 1,103.5 | 2,189.0 | 2,188.0 | 18 |
| 10 | 1,331.5 | 666.3 | 1,314.5 | 1,313.5 | W | 2,103.0 | 1,052.0 | 2,085.9 | 2,085.0 | 17 |
| 11 | 1,512.5 | 756.8 | 1,495.5 | 1,494.5 | T+80 | 1,916.9 | 958.9 | 1,899.9 | 1,898.9 | 16 |
| 12 | 1,675.6 | 838.3 | 1,658.6 | 1,657.6 | $Y$ | 1,735.9 | 868.4 | 1,718.8 | 1,717.9 | 15 |
| 13 | 1,790.6 | 895.8 | 1,773.6 | 1,772.6 | D | 1,572.8 | 786.9 | 1,555.8 | 1,554.8 | 14 |
| 14 | 1,889.7 | 945.3 | 1,872.7 | 1,871.7 | Y | 1,457.8 | 729.4 | 1,440.8 | 1,439.8 | 13 |
| 15 | 2,018.7 | 1,009.9 | 2,001.7 | 2,000.7 | E | 1,358.7 | 679.9 | 1,341.7 | 1,340.7 | 12 |
| 16 | 2,132.8 | 1,066.9 | 2,115.7 | 2,114.8 | N | 1,229.7 | 615.3 | 1,212.6 | 1,211.7 | 11 |
| 17 | 2,288.9 | 1,144.9 | 2,271.8 | 2,270.9 | R | 1,115.6 | 558.3 | 1,098.6 | 1,097.6 | 10 |
| 18 | 2,385.9 | 1,193.5 | 2,368.9 | 2,367.9 | P | 959.5 | 480.3 | 942.5 | 941.5 | 9 |
| 19 | 2,442.9 | 1,222.0 | 2,425.9 | 2,424.9 | G | 862.5 | 431.7 | 845.5 | 844.5 | 8 |
| 20 | 2,590.0 | 1,295.5 | 2,573.0 | 2,572.0 | F | 805.5 | 403.2 | 788.4 | 787.4 | 7 |
| 21 | 2,661.0 | 1,331.0 | 2,644.0 | 2,643.0 | A | 658.4 | 329.7 | 641.4 | 640.4 | 6 |
| 22 | 2,732.1 | 1,366.5 | 2,715.1 | 2,714.1 | A | 587.4 |  | 570.3 | 569.3 | 5 |
| 23 | 2,831.2 | 1,416.1 | 2,814.1 | 2,813.1 | Y | 516.3 |  | 499.3 | 498.3 | 4 |
| 24 | 2,960.2 | 1,480.6 | 2,943.2 | 2,942.2 | E | 417.2 |  | 400.2 | 399.2 | 3 |
| 25 | 3,073.3 | 1,537.1 | 3,056.3 | 3,055.3 | L | 288.2 |  | 271.2 |  | 2 |
| 26 | 3,247.4 | 1,624.2 | 3,230.4 | 3,229.4 | R | 175.1 |  | 158.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| EYVKKQTWNLQGQALEQAIISQKPQLEK | pY | 1084.221 | 3249.6412 | 3 | 3249.6434 | -0.0023 | 45.43 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 130.0 |  |  | 112.0 | E | 3,250.7 | 1,625.8 | 3,233.6 | 3,232.6 | 27 |
| 2 | 373.1 |  |  | 355.1 | Y+80 | 3,121.6 | 1,561.3 | 3,104.6 | 3,103.6 | 26 |
| 3 | 472.1 |  |  | 454.1 | 7 | 2,878.6 | 1,439.8 | 2,861.6 | 2,860.6 | 25 |
| 4 | 600.2 | 300.6 | 583.2 | 582.2 | K | 2,779.5 | 1,390.3 | 2,762.5 | 2,761.5 | 24 |
| 5 | 728.3 | 364.7 | 711.3 | 710.3 | Q | 2,651.4 | 1,326.2 | 2,634.4 | 2,633.4 | 23 |
| 6 | 829.3 | 415.2 | 812.3 | 811.3 | T | 2,523.4 | 1,262.2 | 2,506.3 | 2,505.3 | 22 |
| 7 | 1,015.4 | 508.2 | 998.4 | 997.4 | W | 2,422.3 | 1,211.7 | 2,405.3 | 2,404.3 | 21 |
| 8 | 1,129.5 | 565.2 | 1,112.4 | 1,111.5 | N | 2,236.2 | 1,118.6 | 2,219.2 | 2,218.2 | 20 |
| 9 | 1,242.6 | 621.8 | 1,225.5 | 1,224.5 | L | 2,122.2 | 1,061.6 | 2,105.2 | 2,104.2 | 19 |
| 10 | 1,370.6 | 685.8 | 1,353.6 | 1,352.6 | Q | 2,009.1 | 1,005.1 | 1,992.1 | 1,991.1 | 18 |
| 11 | 1,427.6 | 714.3 | 1,410.6 | 1,409.6 | G | 1,881.0 | 941.0 | 1,864.0 | 1,863.0 | 17 |
| 12 | 1,555.7 | 778.4 | 1,538.7 | 1,537.7 | Q | 1,824.0 | 912.5 | 1,807.0 | 1,806.0 | 16 |
| 13 | 1,626.7 | 813.9 | 1,609.7 | 1,608.7 | A | 1,696.0 | 848.5 | 1,678.9 | 1,678.0 | 15 |
| 14 | 1,739.8 | 870.4 | 1,722.8 | 1,721.8 | L | 1,624.9 | 813.0 | 1,607.9 | 1,606.9 | 14 |
| 15 | 1,868.9 | 934.9 | 1,851.8 | 1,850.8 | E | 1,511.8 | 756.4 | 1,494.8 | 1,493.8 | 13 |
| 16 | 1,996.9 | 999.0 | 1,979.9 | 1,978.9 | Q | 1,382.8 | 691.9 | 1,365.8 | 1,364.8 | 12 |
| 17 | 2,068.0 | 1,034.5 | 2,050.9 | 2,049.9 | A | 1,254.7 | 627.9 | 1,237.7 | 1,236.7 | 11 |
| 18 | 2,181.0 | 1,091.0 | 2,164.0 | 2,163.0 | I | 1,183.7 | 592.4 | 1,166.7 | 1,165.7 | 10 |
| 19 | 2,294.1 | 1,147.6 | 2,277.1 | 2,276.1 | I | 1,070.6 | 535.8 | 1,053.6 | 1,052.6 | 9 |
| 20 | 2,381.2 | 1,191.1 | 2,364.1 | 2,363.1 | S | 957.5 | 479.3 | 940.5 | 939.5 | 8 |
| 21 | 2,509.2 | 1,255.1 | 2,492.2 | 2,491.2 | Q | 870.5 | 435.8 | 853.5 | 852.5 | 7 |
| 22 | 2,637.3 | 1,319.2 | 2,620.3 | 2,619.3 | K | 742.4 | 371.7 | 725.4 | 724.4 | 6 |
| 23 | 2,734.4 | 1,367.7 | 2,717.3 | 2,716.3 | P | 614.4 |  | 597.3 | 596.3 | 5 |
| 24 | 2,862.4 | 1,431.7 | 2,845.4 | 2,844.4 | Q | 517.3 |  | 500.3 | 499.3 | 4 |
| 25 | 2,975.5 | 1,488.3 | 2,958.5 | 2,957.5 | L | 389.2 |  | 372.2 | 371.2 | 3 |
| 26 | 3,104.5 | 1,552.8 | 3,087.5 | 3,086.5 | E | 276.2 |  | 259.1 | 258.1 | 2 |
| 27 | 3,250.7 | 1,625.8 | 3,233.6 | 3,232.6 | K | 147.1 |  | 130.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| KSSPAQGNR | pS | 512.7313 | 1023.448 | 2 | 1023.4498 | -0.0018 | 35.51 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 129.1 | 65.1 | 112.1 |  | K | 1,024.5 | 512.7 | 1,007.4 | 1,006.4 | 9 |
| 2 | 216.1 | 108.6 | 199.1 | 198.1 | S | 896.4 | 448.7 | 879.3 | 878.4 | 8 |
| 3 | 383.1 | 192.1 | 366.1 | 365.1 | S+80 | 809.3 | 405.2 | 792.3 | 791.3 | 7 |
| 4 | 480.2 | 240.6 | 463.2 | 462.2 | P | 642.3 | 321.7 | 625.3 |  | 6 |
| 5 | 551.2 | 276.1 | 534.2 | 533.2 | A | 545.3 |  | 528.3 |  | 5 |
| 6 | 679.3 | 340.1 | 662.3 | 661.3 | Q | 474.2 |  | 457.2 |  | 4 |
| 7 | 736.3 | 368.7 | 719.3 | 718.3 | G | 346.2 |  | 329.2 |  | 3 |
| 8 | 850.3 | 425.7 | 833.3 | 832.3 | N | 289.2 |  | 272.1 |  | 2 |
| 9 | 1,024.5 | 512.7 | 1,007.4 | 1,006.4 | R | 175.1 |  | 158.1 |  | 1 |


| Sequence | Modification | Exp. m/z | Exp. M.W. | Charge | Cal. M.W. | Delta | Score |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| EALPMDTEVYESPYADPEEIRPK | Mox; 2 pY | 952.3976 | 2854.171 | 3 | 2854.1697 | 0.0013 | 60.41 |



| B | B Ions | $\mathrm{B}+2 \mathrm{H}$ | B-NH3 | B-H2O | AA | Y Ions | $\mathrm{Y}+2 \mathrm{H}$ | Y-NH3 | Y-H2O | Y |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 130.0 |  |  | 112.0 | E | 2,855.2 | 1,428.1 | 2,838.2 | 2,837.2 | 23 |
| 2 | 201.1 |  |  | 183.1 | A | 2,726.1 | 1,363.6 | 2,709.1 | 2,708.1 | 22 |
| 3 | 314.2 |  |  | 296.2 | L | 2,655.1 | 1,328.1 | 2,638.1 | 2,637.1 | 21 |
| 4 | 411.2 |  |  | 393.2 | P | 2,542.0 | 1,271.5 | 2,525.0 | 2,524.0 | 20 |
| 5 | 558.3 |  |  | 540.2 | M+16 | 2,445.0 | 1,223.0 | 2,427.9 | 2,427.0 | 19 |
| 6 | 673.3 | 337.1 |  | 655.3 | D | 2,297.9 | 1,149.5 | 2,280.9 | 2,279.9 | 18 |
| 7 | 774.3 | 387.7 |  | 756.3 | T | 2,182.9 | 1,092.0 | 2,165.9 | 2,164.9 | 17 |
| 8 | 903.4 | 452.2 |  | 885.4 | E | 2,081.9 | 1,041.4 | 2,064.8 | 2,063.8 | 16 |
| 9 | 1,002.4 | 501.7 |  | 984.4 | Y | 1,952.8 | 976.9 | 1,935.8 | 1,934.8 | 15 |
| 10 | 1,245.5 | 623.2 |  | 1,227.5 | Y+80 | 1,853.7 | 927.4 | 1,836.7 | 1,835.7 | 14 |
| 11 | 1,374.5 | 687.8 |  | 1,356.5 | E | 1,610.7 | 805.9 | 1,593.7 | 1,592.7 | 13 |
| 12 | 1,461.5 | 731.3 |  | 1,443.5 | S | 1,481.7 | 741.3 | 1,464.6 | 1,463.7 | 12 |
| 13 | 1,558.6 | 779.8 |  | 1,540.6 | P | 1,394.6 | 697.8 | 1,377.6 | 1,376.6 | 11 |
| 14 | 1,801.6 | 901.3 |  | 1,783.6 | Y+80 | 1,297.6 | 649.3 | 1,280.6 | 1,279.6 | 10 |
| 15 | 1,872.7 | 936.8 |  | 1,854.7 | A | 1,054.6 | 527.8 | 1,037.5 | 1,036.5 | 9 |
| 16 | 1,987.7 | 994.4 |  | 1,969.7 | D | 983.5 | 492.3 | 966.5 | 965.5 | 8 |
| 17 | 2,084.7 | 1,042.9 |  | 2,066.7 | P | 868.5 | 434.7 | 851.5 | 850.5 | 7 |
| 18 | 2,213.8 | 1,107.4 |  | 2,195.8 | E | 771.4 | 386.2 | 754.4 | 753.4 | 6 |
| 19 | 2,342.8 | 1,171.9 |  | 2,324.8 | E | 642.4 | 321.7 | 625.4 | 624.4 | 5 |
| 20 | 2,455.9 | 1,228.5 |  | 2,437.9 | I | 513.4 | 257.2 | 496.3 |  | 4 |
| 21 | 2,612.0 | 1,306.5 | 2,595.0 | 2,594.0 | R | 400.3 | 200.6 | 383.2 |  | 3 |
| 22 | 2,709.1 | 1,355.0 | 2,692.0 | 2,691.1 | P | 244.2 |  | 227.1 |  | 2 |
| 23 | 2,855.2 | 1,428.1 | 2,838.2 | 2,837.2 | K | 147.1 |  | 130.1 |  | 1 |

## Supplementary figure 1

## Annotated ESI-MSMS spectra of phosphorylated tryptic peptides derived from

 Syk.Annotated Mascot MSMS spectra of phosphopeptides are shown and the corresponding assigned fragment ions. The table above the spectra lists the $\mathrm{m} / \mathrm{z}$ values of the precursor ions, the charge state, the corresponding MW, the mass deviation, the peptide score (in MASCOT), the confirmed phosphorylation site, the identified sequence and the modification(s) of the sequenced peptide. Spectra were recorded on an Orbitrap MS (Thermo Fisher Scientific). The precursor in MS showed a mass accuracy of $\leq 2 \mathrm{ppm}$. At least one MSMS spectrum is shown for each p-site.

## A



B




## Supplementary figure 2

Growth curves of KG-1-, FFM05- and FFM12 cells that were left untreated/DMSO treated (black lines) or were treated (A) with the Src kinase inhibitor pp2 at a final concentration of $1 \mu \mathrm{M}$ (grey lines) or (B) with Dasatinib at a final concentration of 4 nM (grey lines). Proliferation was monitored by an XTT-based assay as outlined in the Methods section.


## Supplementary figure 3

(A) Schematic representation of the FGFR1OP2-FGFR1 fusion protein. (B) RT-PCR of the fusion region of the FGFR1OP2-FGFR1 fusion protein. The following primers were used: forward ATCAGTCGGCCTTGGAACTTA, reverse AGAAGAACCCCAGAGTTCATG (C) 48 hours after silencing of FGFR1, KG-1 cells were harvested and lysed. The respective lysates were subjected to immunoblot analysis using antibodies against FGFR1, pSTAT3, pSTAT5, pSyk and actin. (D) Growth curve of KG-1 cells that were treated with shRNAs against FGFR1 (grey line) or the respective control shRNAs (black line). Proliferation was monitored by an XTT-based assay.

| UPN | Age | AML sec. to | WBC $\times 10^{9} / \mathrm{L}$ <br> (\% blasts) | Karyotype | Molecular-genetic findings | Risk group |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| FFM05 | 60 | MDS | $2 \text { (7\%) }$ <br> BM: 25\% | At onset: 4445,XY,t(1;3)(q4 2;q27), <br> del(5)(q14q33)- <br> 7, del(16)(q23),+ <br> MAI1,+Mar2 | None (No FLT3-ITD mutations, no FLT3-kinase domain mutations, no Kit mutations) | HR |
| FFM12 | 24 | - | 7 (22\%) | $\begin{aligned} & 45, X X,-7[12] \\ & 46, X X[8] \end{aligned}$ | AML1/ETO; NRAS (No FLT3-ITD mutations, no FLT3-kinase domain mutations, no Kit mutations) | HR |

## Supplementary table 1:

## Primary AML patient characteristics.

Primary AML cells of two patients were purified and cultured as outlined in the Material and Methods section and the respective primary AML cell lines are denominated as FFM05 and FFM12. Enlisted are the results of the cytogenetic and molecular-genetic analyses, the age of the patients, the initial white blood count (WBC) and the respective risk groups.

| AML-specific <br> p-sites | B cell-specific <br> p-sites |
| :---: | :---: |
| S3/4 | Y28 |
| S9 | S44 |
| Y389 | T256 |
| S443 | S306 |
| T610 | S316 |
| - | T317 |
| - | S319 |
| - | S379 |
| - | T384 |
| - | T530 |
| - | S579 |
| - | T582 |

## Supplementary table 3:

Cell type-specific phosphorylation patterns.
P-sites that were identified in AML cells and were not reported to be phosphorylated in B cells are outlined in the left column. P-sites that were previously identified in B cell antigen receptor stimulated $B$ cells but not in AML cells are listed in the right column ${ }^{26}$.

